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C. Galle, L. Dupuy, T. Jourdan, L. Gélébart. Prediction of nuclear materials behavior for reactors life-span extension towards a multi-scale approach dedicated to microstructure and mechanical properties of irradiated materials. NuMat 2018, Oct 2018, Seattle, United States. cea-02338707

HAL Id: cea-02338707

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Submitted on 24 Feb 2020

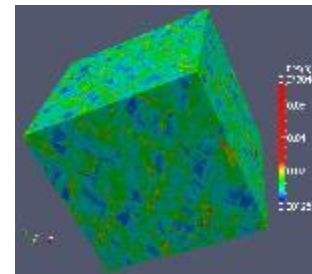
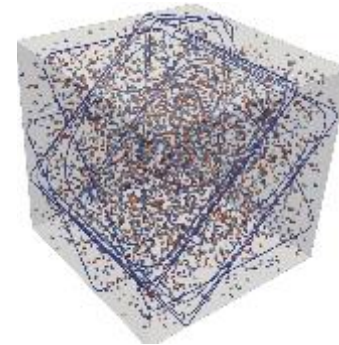
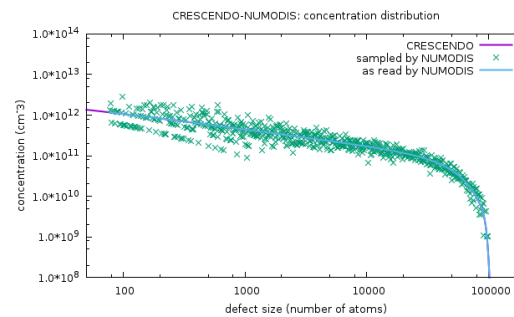
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DE LA RECHERCHE À L'INDUSTRIE



Prediction of nuclear materials behavior for reactors life-span extension: towards a multiscale approach dedicated to microstructure and mechanical properties of irradiated materials



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CEA Saclay, France
Nuclear Energy Division/Department of Nuclear Materials

Structural and in-core materials in NPP are submitted to severe conditions due to coupled thermal, irradiation, mechanical, chemical solicitations

Life-span extension (at least 60/80 y), safety increase and, economical model optimization rely on material ageing studies of key components supported by simulation

Nuclear studies implies an extremely large number of physical and chemical mechanisms from early primary neutron damages (~ 10 nm / ~ 1 ns) to macroscopical properties (~ 1 mm) after several decades (40 y) of operating reactor

Intrinsically, ageing mechanisms understanding and temperature and neutron irradiation effects prediction need a multiscale/multiphysics approach

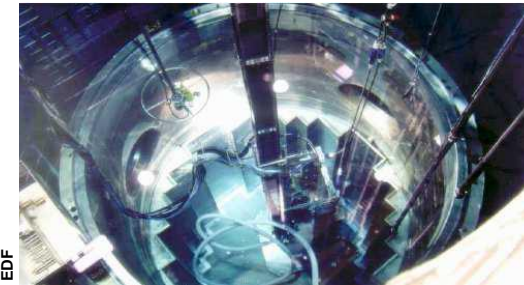
Progress in material sciences & numerical simulation, allow now to address such topics with less empirical tools using more and more physical models

PWR (EPR) reactor pressure vessel



EDF

RPV Lower internals



EDF

Fuel cladding after pressure tests



CEA

In France, as in many European countries, there is no operation time limit for nuclear reactors but there is an obligation (L. 593-18 article from the environment code) for the operators to:

- ☞ **1:** deeply examine, every ten years, the conformity of their installation with the legal & applicable reference
- ☞ **2:** address potential detected gaps and optimize their periodical level
- ☞ **3:** thoroughly review the ageing effects on materials

Reactors life-span extension, a significant step

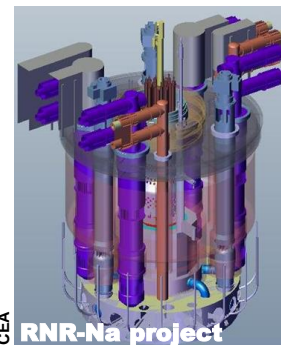
- In the future, current reactors will coexist with EPR or equivalent new type, or GenIV FNR reactors with upgraded safety requirements
- Current reactors operating over the initial duration will require:
 - To revise the safety demonstration and improve the safety
 - To demonstrate that the ageing of key equipment is well managed
 - To replace some equipment

Example of key issues (life-span extension at least up to 60 y)

- Behavior of the RPV (and internals) with an extra irradiation dose (+50%) and, consequently, the ageing management
- Ageing management of the concrete confinement building
- Electric cables ageing investigation



EPR Flamenville reactors with new EPR

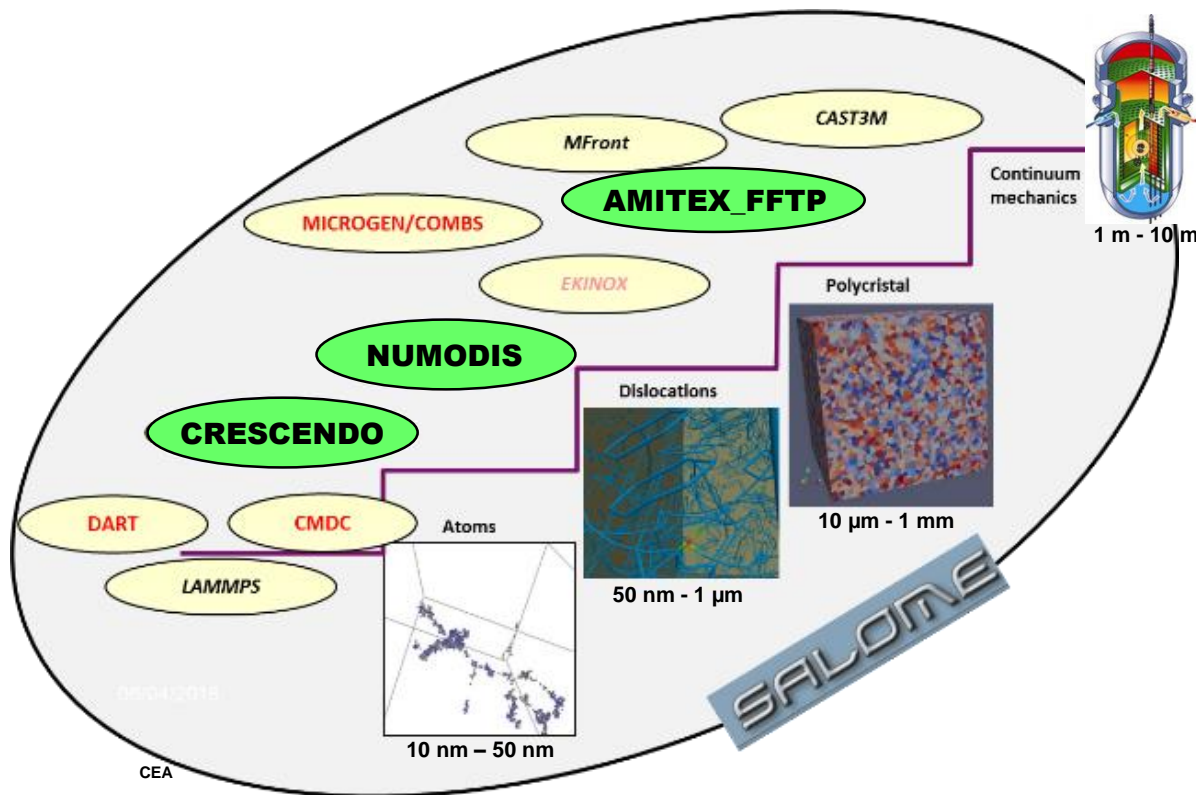


CEA RNR-Na project

The MATIX_P platform, a tool to implement a multiphysics/multiscale approach for irradiated nuclear materials

MATIX_P, a multiscale numerical simulation platform

- Gathering a set of calculation codes dedicated to materials microstructure and mechanical properties evolution prediction after irradiation
- Allowing data exchange between codes, codes chaining/coupling with a unified work environment (Graphic user interface)
- Based on codes content ownership (self development or Open-source tools ownership) and on the SALOME Open-source software for pre/post-processing



MATIX

SALOME

MICROGEN

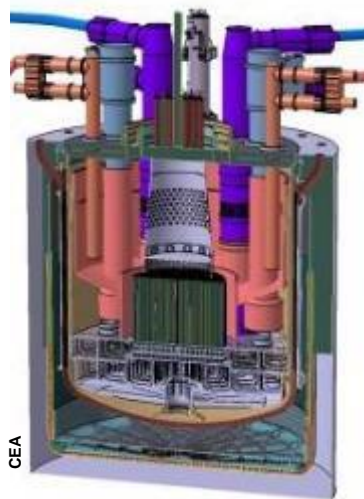


The MATIX_P platform is part of the basic research strategy, dedicated to industrial issues

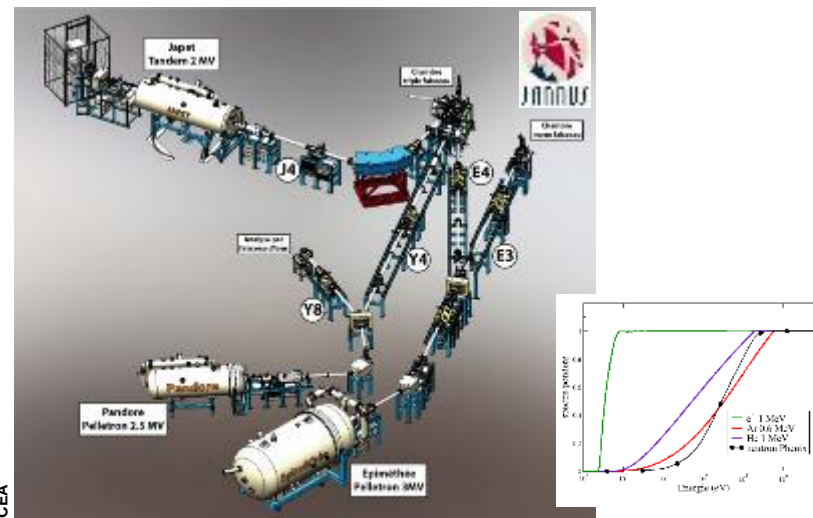
- ☞ **Line 1:** prediction of the hardening kinetics of current PWR RPV steel (bainite) under irradiation
- ☞ **Line 2:** prediction of thermal and irradiation creep of austenitic steels (SFR vessel and structures)
- ☞ **Line 3:** use of numerical tools allowing the comparison of ion and neutron irradiation damages to support the CEA JANNuS irradiation platform development



PWR



SFR

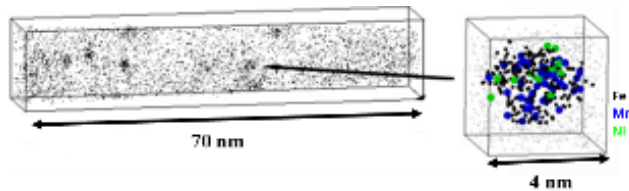


JANNuS ion irradiation platform (CEA Saclay)



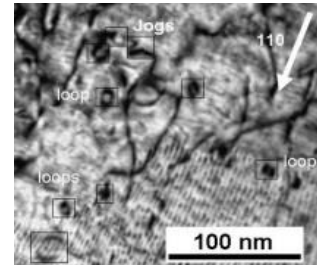
A multiphysics and multiscale issue

Microstructure



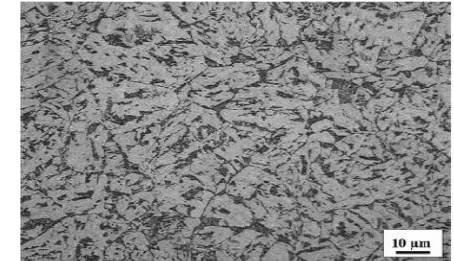
E. Meslin *et al.* (2010)

Clusters in irradiated (neutron) FeMnNi model alloy



C. Robertson *et al.* (2008)

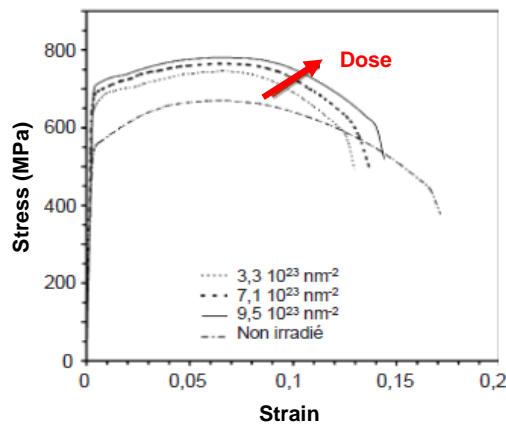
Dislocation loops in irradiated (ion) pure iron



Hausild *et al.* (2002)

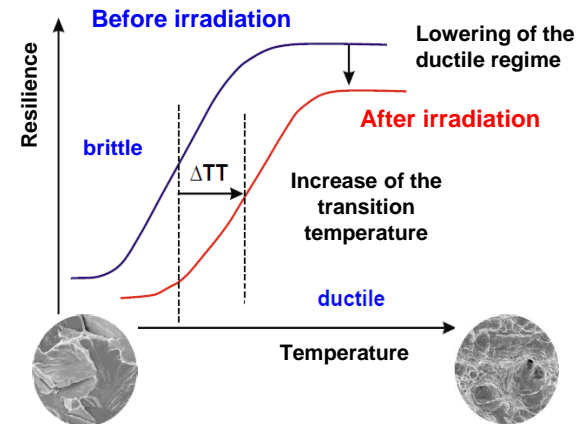
Bainite (RPV steel) initial microstructure

Mechanical properties



Hausild *et al.* (2002)

Tensile curve for a low-alloyed steel



Raoul *et al.* (1999)

Temperature Ductile Brittle Transition (TDBT) curve evolution

Scientific goal

- ☞ Prediction of the hardening induced by irradiation of a monocrystal model alloy from initial nanostructure and later extended to polycrystal (REV)

Applicative goal

- ☞ Step by step implementation of the multiscale approach

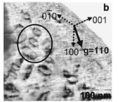
Main goals for the platform

- ☞ Demonstration of the feasibility and relevance of the multiscale approach
- ☞ Achievement of the chaining of CRESCENDO, NUMODIS and AMITEX_FFTP codes

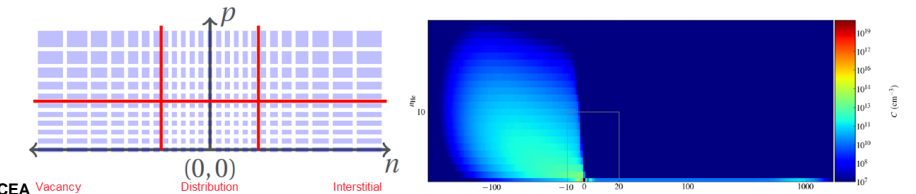
CRESCENDO, cluster dynamics Code



- **Goal:** calculation of irradiation induced microstructure for an extended period of time
- **Method:** mean field approach with chemical kinetics equation
- **Key parameter:** irradiation defects concentration (loops, He bubbles...)



$$\frac{dC_{(n,p)}}{dt} = - \underbrace{\sum_{(m,q)} \beta_{(n,p),(m,q)} C_{(n,p)} C_{(m,q)} + \dots}_{\text{Flux between species}} + \underbrace{G_{(n,p)}}_{\text{irradiations}} - \underbrace{k_{(n,p)} (C_{(n,p)} - \bar{C}_{(n,p)})}_{\text{Dislocations, grain boundary...}}$$

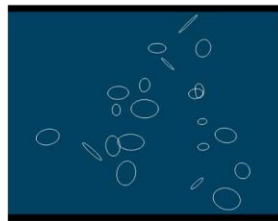


CEA Vacancy Distribution Interstitial
T. Jourdan et al., "An accurate scheme to solve cluster dynamics equations using a Fokker-Planck approach", *Computer Physics Communications* 207 (2016) 170-178

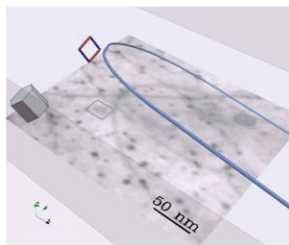
NUMODIS, Dislocation dynamics Code



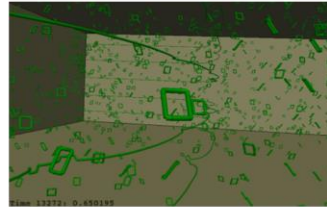
- **Goal:** modeling and understanding of a monocrystal mechanical behavior through the dislocation collective behavior
- **Method:** dislocations dynamics
- **Key parameters:** dislocations, grain boundary, precipitates, irradiation defects



B. Bako, E. Clouet et al. (2009)



J. Drouet et al. (2016)



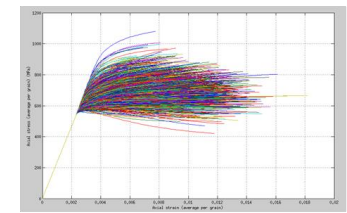
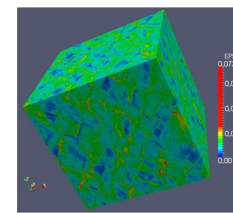
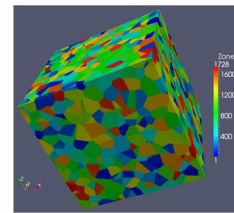
A. Etcheverry et al. (2015)

CEA

X. Shi, L. Dupuy et al., "Interaction of 100 dislocation loops with dislocations studied by dislocation dynamics in alpha-iron", *Journal of Nuclear Materials*, 2015, 460, 37-43

AMITEX Code, FFT method

- **Goal:** mechanical behavior simulation of a REV from a crystalline plasticity law
- **Method:** aggregate calculation through FFT method FFT
- **Key parameters:** crystalline plasticity law, microstructure...



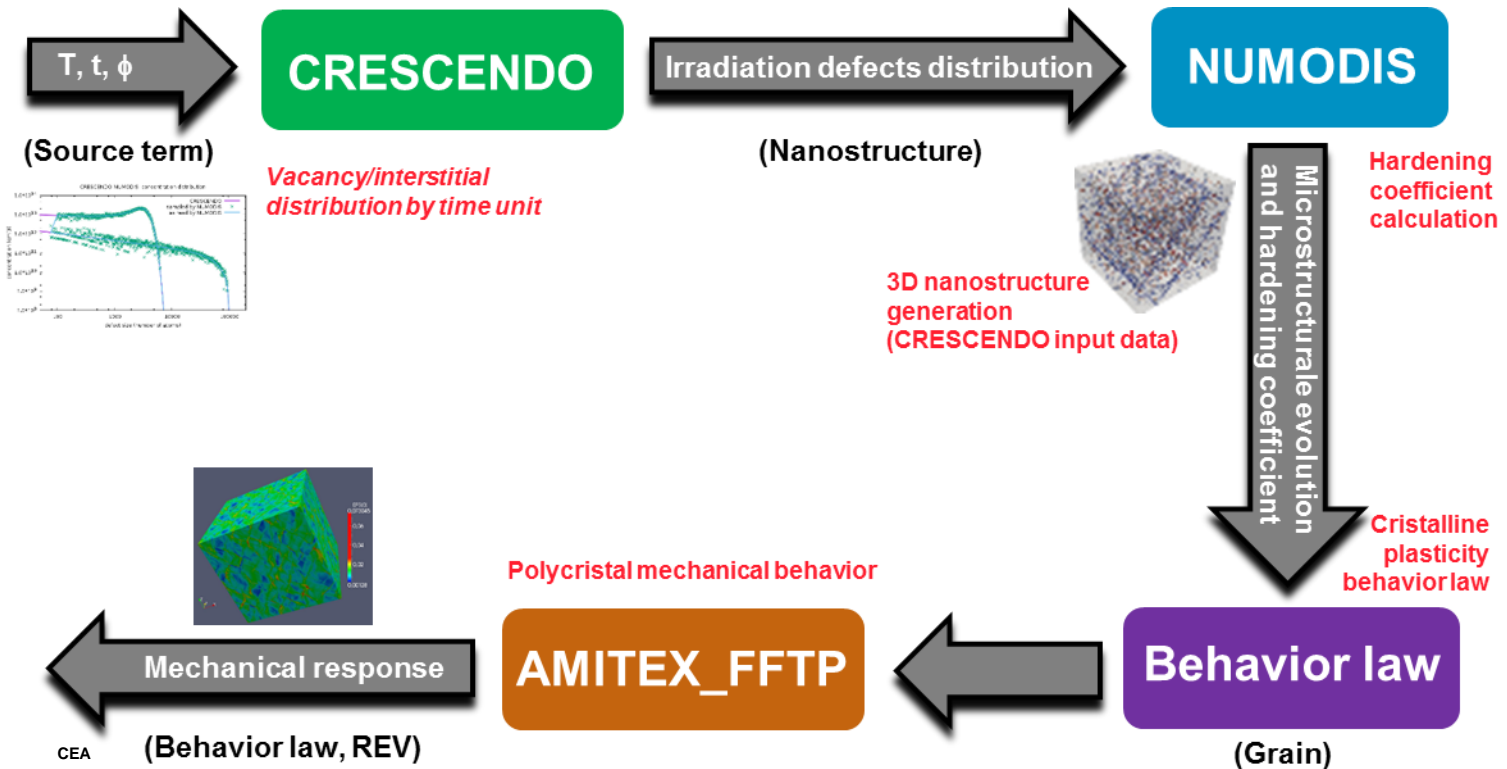
1728 grains (12x12x12), ~22x22x22 points / grain, ~100 millions DDL with BCC crystalline law (HPP), ~50 internal variables (L. Gélébart)

CEA

L. Gélébart & R. Mondon-Cancel, "Non-linear extension of FFT-based methods accelerated by conjugate gradients to evaluate the mechanical behavior of composite materials", *Computational Materials Science* 77 (2013) 430-439

CRESCENDO, NUMODIS & AMITEX_FFTP codes chaining: from nanostructure, to mechanical properties at grain scale up to polycrystal

A multiscale approach implemented by the chaining of the main codes of MATIX_P platform



CRESCENDO

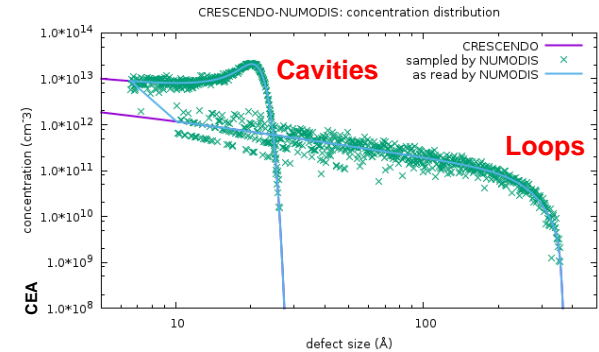
Input data

- Dose, time, temperature, material parameters

Outlet data

- Size distribution of defects (loops, cavities) in homogeneous media

Distribution of nano-defects (interstitial loops & cavities) calculated by the CRESCENDO code



NUMODIS

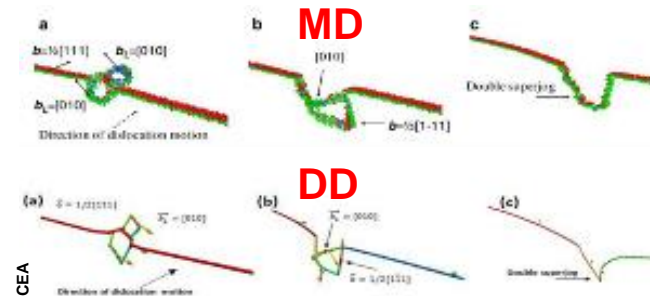
A DD code used to study the plastic deformation of materials based on the collective behavior of dislocations and to calculate the mechanical behavior at grain scale

Input data

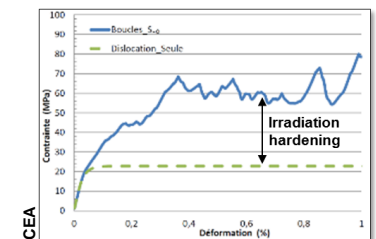
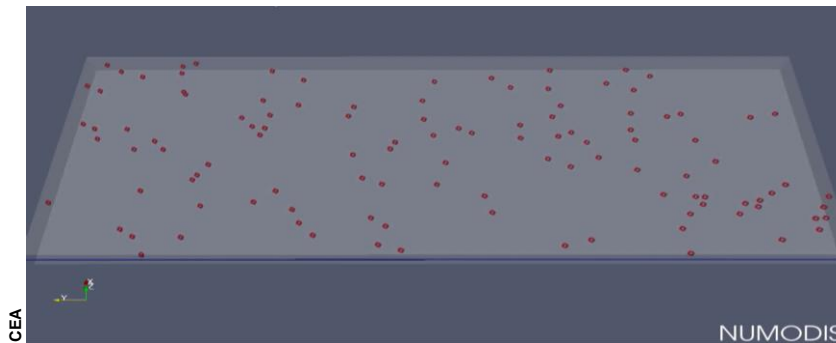
- Mechanical loading, initial nanostructure, material parameters

Outlet data

- Evolution of the microstructure during the deformation stage
- Mechanical behavior of the simulated domain



Dislocations line interaction with nanodefects simulated with NUMODIS code



Dislocations/defects interaction: stress/strain tensile curve


Generation of 3D nanostructure by NUMODIS DD code from the defects distribution (size, nature, density) calculated by CRESCENDO CD code (irradiated model material: ferrite)

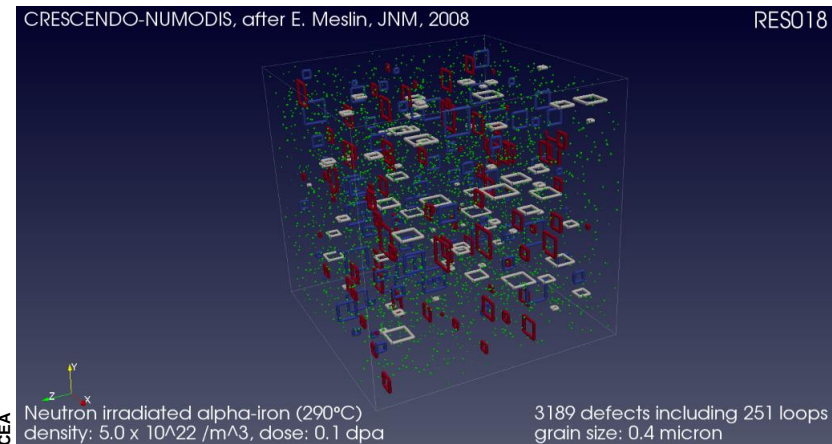
- ☞ **1 step:** random sampling of the defects distribution provided by CRESCENDO
- ☞ **2 step:** random positioning of the sampled defects without overlapping
- ☞ **3 step:** reconstruction of the nanostructure

Accounted defects

- BCC material (ex. RPV steel): $\langle 100 \rangle$, $\frac{1}{2} \langle 111 \rangle$ loops, cavities
- FCC material (austenitic steels, internals): Frank loops, cavities
- HCP material (Zr alloys, cladding): $\langle a \rangle$, $\langle c \rangle$ loops, cavities

Standard outlet

- Reconstruction of the nanostructure and visual display with Para view visualization tool  Parallel Visualization Application
- Random positioning of the defects (no overlapping)
- Reconstruction of the microstructure



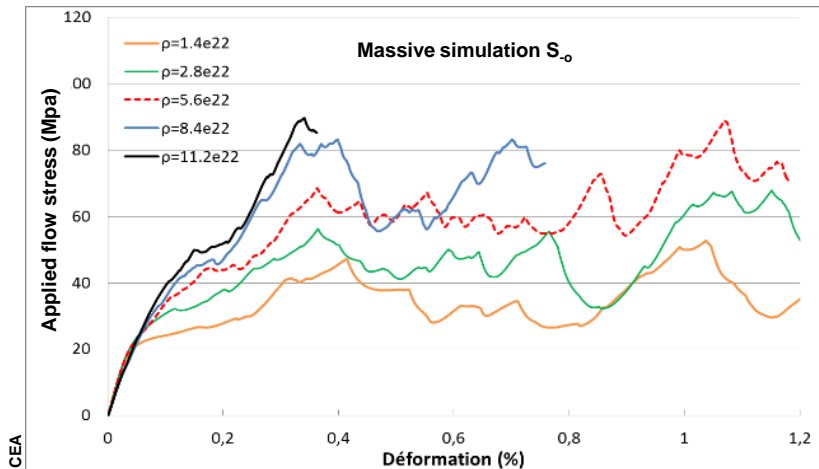
**Reconstructed microstructure with nano-defects
($\langle 100 \rangle$ loops in different plans and cavities)
calculated by NUMODIS with CRESCENDO data
(0.1 dpa neutron irradiation, 0.4 μm iron grain)**

Establishment of the mechanical properties evolution of irradiated materials at macroscopic scale, using a multiscale approach, require the identification of cristalline plasticity law

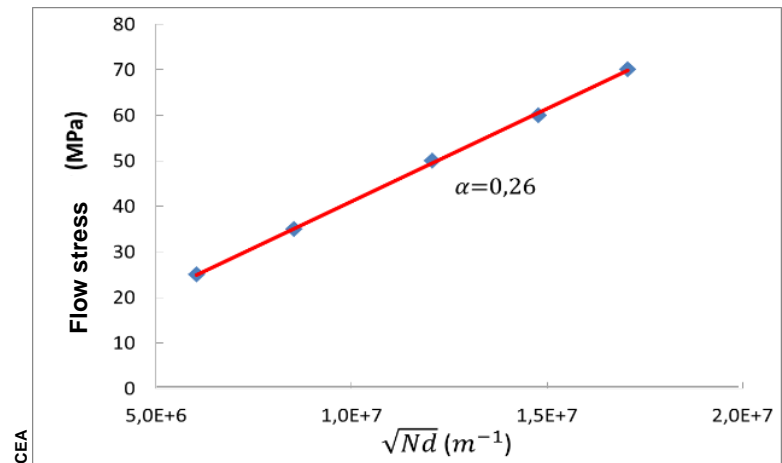
From DD calculations at the grain scale, different steps are considered:

- Retrieving of the relevant parameters (elastic coefficients, flow law, dislocations viscosity...), for the cristalline plasticity law issued from DD calculations (grain scale)
- Introduction of cristalline plasticity law (Orowan formalism) with the tool generator MFRONT
- Retrieving of the physical relevant parameters
 - Coefficient of the hardness matrix
 - Hardening coefficients

$$\Delta\tau = \alpha\mu b(Nd)^{1/2}$$



Influence of the loops size and density on the hardening



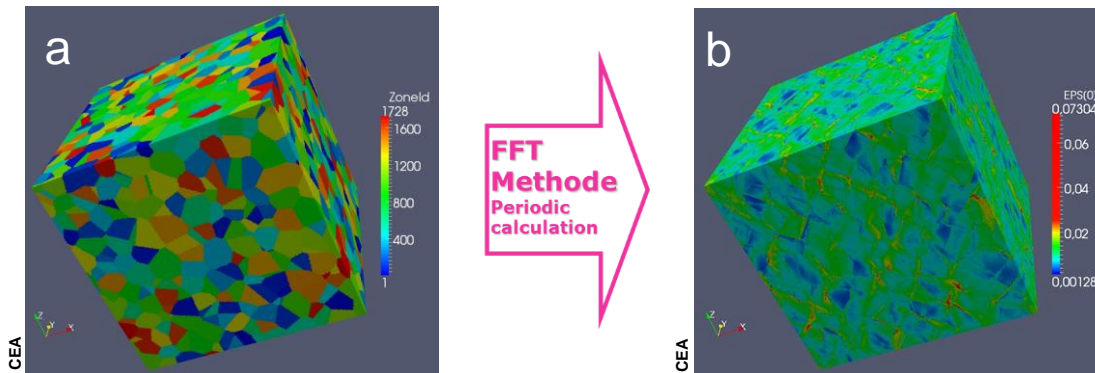
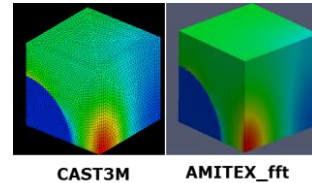
Orowan formalism and introduction of the cristalline plasticity law

AMITEX_FFTP <http://www.maisondelasimulation.fr/projects/amtex/html/overview.html>

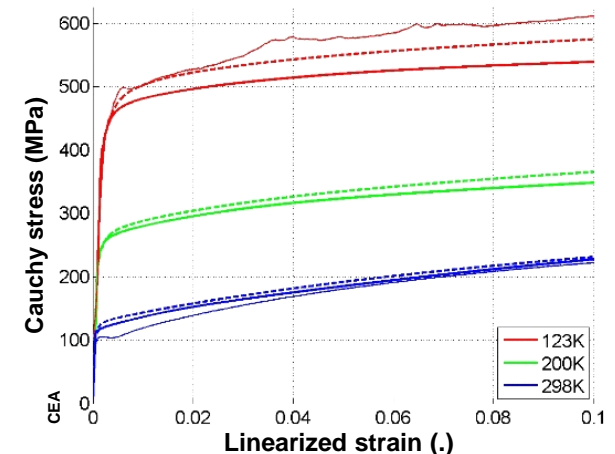
- A new FFT code (solver), highly parallelized, used to simulate the non-linear mechanical behavior of unit-cells representative of heterogeneous materials

Compared to conventional FE codes → no-mesh, greater efficiency, easy implementation, well-suited for parallelization

- For metallic alloys, it corresponds to crystalline aggregates for which the behavior of each grain is based on dislocation dynamics modeling and has been experimentally validated
- The method links the behavior of one grain ($\approx 10 \mu\text{m}$) to that of a representative elementary volume (polycrystal), REV ($\approx 100 \mu\text{m} - 1 \text{mm}$)
- Method
 - Aggregate calculation using FFT method
- Key parameters
 - Crystalline plasticity law, microstructure



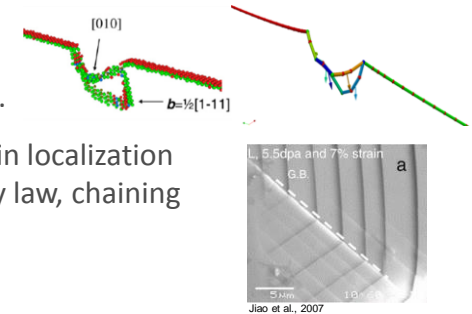
a) Voronoï microstructure used to calculate the mechanical behavior of a BCC iron polycrystal (≈ 1728 grains) and **b)** reconstruction of stress distribution (axial strain heterogeneities)



Tensile curve for an iron polycrystal: experiences (- - -) and AMITEX_FFTP (—) simulation fit

■ Main results

- A multiscale/multiphysics approach if relevant to address the evolution of irradiated materials (metallic alloys) mechanical properties
- The successful achievement of a first chaining of the codes CRESCENDO, NUMODIS and AMITEX_FFTP allowed to link irradiation induced microstructure to the behavior of a reference elementary volume (REV), representative of an heterogeneous material unit-cell
- Nevertheless, in the context of RPV steel application, improvement of physical models is necessary:
 - **CRESCENDO code:** better parameterization and validation
 - **NUMODIS code:** accounting of alloys effects (chemistry), interaction of screw dislocations with cavities and loops, temperature effect, small clusters effects...
 - **AMITEX_FFTP code:** accounting of more complex microstructures and of strain localization (grain boundaries/clear bands interaction), use of stabilized crystalline plasticity law, chaining with CAST3M numerical simulation tool used in structural mechanics



■ Remaining key issues

- Industrial materials complexity at the different time and space scales, reduces yet the possibility to substitute the multiscale approach to the configuration experiences + semi-empirical models
- Experimental validation: essential whatever the scales
- Remaining scientific locks
 - Limitation of the physical models used
 - Input data uncertainties for the models
 - Scales overlapping and intermediate models relevancy for information transmission
 - Numerical locks: increasing complexity of models and codes, parallelization

Acknowledgements

**L. Dupuy, T. Jourdan, L. Gélébart, L. Vincent,
M. Shukeir et al. (CEA/DEN/DMN)**

C. Bourcier, C. Van Wambeke (CEA/DEN/DM2S)

J. Derouillat (CEA/Maison de la simulation)

G. Adjanor, G. Monnet (EDF)

B. Devindre (CNRS/ONERA)

**And thank you all for
your attention**