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# THE MATERIALS AGEING PLATFORM : TOWARDS A TOOLBOX TO PERFORM A WIDE RANGE OF RESEARCH STUDIES ON THE BEHAVIOUR OF INDUSTRIAL MATERIALS

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**ABSTRACT:** This paper presents the Materials Ageing Platform developed at EDF R&D, whose objective is to perform studies on the behaviour of industrial materials using advanced experimental and modeling techniques. We will focus on multi-scale modeling approaches relying on some recent development of the platform, allowing the study of concrete, austenitic steels and bainitic steels. The validation of models from experimental data will take advantage of the development of field measurements at the scale of the microstructure using digital image correlation.

## 1. INTRODUCTION : AN OVERVIEW OF THE PLATFORM IN RELATION WITH CURRENT INDUSTRIAL RESEARCH NEEDS

The development of the Materials Ageing Platform (MAP) has started in 2011 at EDF to reply to an increasing demand of research engineers of multiple tools allowing to study the behaviour of materials using advanced experimental data, multi-scale or multi-physics modelling... Another motivation for developing the platform is to share the developments between an increasing number of researchers active in the field of materials modelling. Indeed, a rapidly expanding number of routines are developed internally at EDF or through partnerships and a high benefit could be gained by sharing them, while saving time by not duplicating efforts. In this document, we will discuss the general objective of the platform and precise the perimeter of tools being integrated, to then present a limited number of recent developments of potentially high impact for research studies.

One of the main motivation of the MAP project is to bridge advanced experimental techniques with modelling and calculations relevant to study concrete and steel alloys used in pressurised water reactors (PWR). Ageing studies rely more and more on multi-scale modelling methods due to their predictive capabilities, especially when thermal or irradiation induced ageing provokes the development of small objects at the micro-structural scale in the case of ferritic materials [1] or micro-structural changes in the case of concrete [2]. Those multi-scale simulations require to derive a micro-structure model from experimental observations [3,4], physically based constitutive equations at the scale of the micro-structure (e.g. crystal plasticity laws [5]), as well as validations relying on the comparison of experimental and calculated mechanical fields at the scale of the microstructure. In this paper, we will first present the recent developments implemented into MAP to generate microstructures, to then present field measurement techniques applied at the micro-structural scale that can be used to validate material behaviour models relevant for such small scales.

## 2. GENERATION OF MICROSTRUCTURES FOR CONCRETE AND AUSTENITIC STEELS

### 2.1. Concrete microstructures

The generation of concrete microstructures was developed during the PhD of J. Escoda [4]. The chosen strategy, calibrated from 3D tomography pictures, considers a multi-scale microstructure composed of a coarse gravel population, a small gravel population, sand and the cement paste. The gravels are modeled as Poisson's polyhedrons. A 2D slice generated using MAP is shown in Figure 1. Such microstructures can be used to perform finite difference volume calculations available in MAP, or Fast-Fourier Transform calculations [6] not yet implemented in MAP.

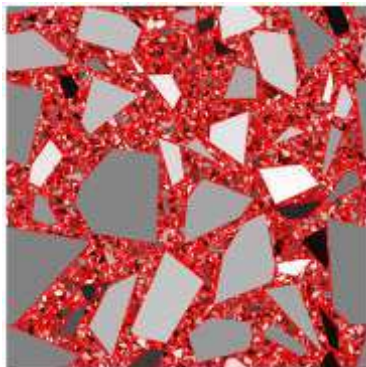
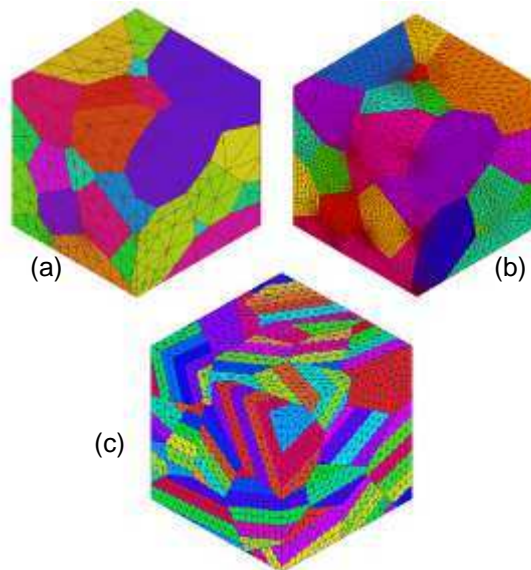


Figure 1- Concrete Microstructure

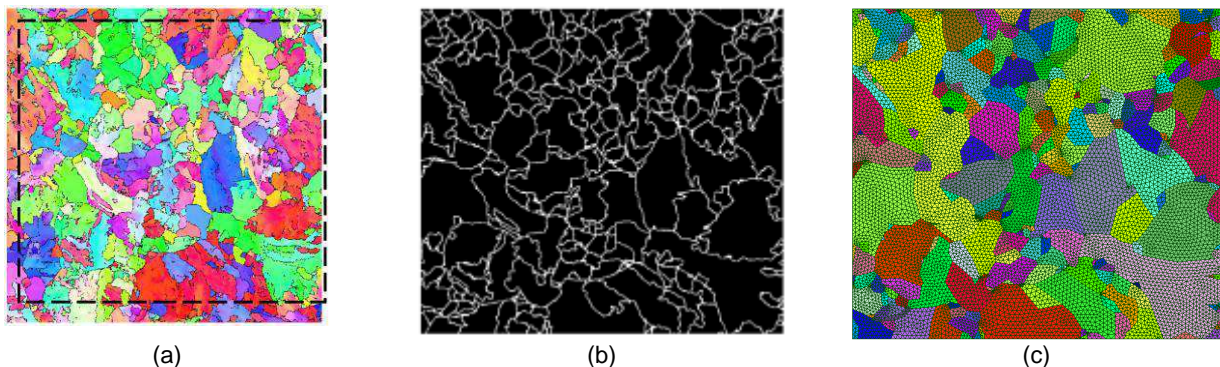
### 2.2. Steel microstructures

The first method, classically employed to generate steel aggregates, consists in using a Voronoi tessellation. From a spatially random distribution of seeds, a collection of convex grains is obtained, quite representative of austenitic steels like AISI 304 and AISI 316 steels used in the core internals of pressurized water reactors, or nickel based steels like alloys 600, 617 or 182 used in various components exposed to corrosion. Once the geometry is created, a parametric automated meshing procedure is performed using the Salome software [7] and produces meshes of chosen coarseness (Fig 2a and 2b). A specific procedure has also been adapted for bainitic microstructures from the work of Osipov et al. [8], considering that the parent austenitic grains are generated using Voronoi polyhedrons then divided into laths (Fig 2c). Such microstructures are relevant for studies of the Reactor Pressure Vessel (RPV) steel.



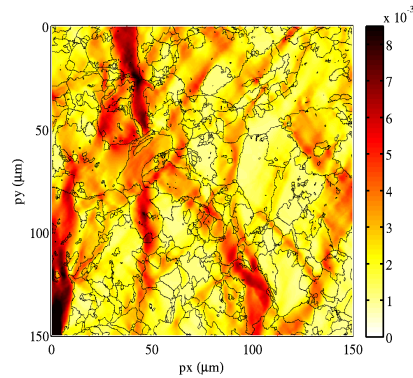
**Figure 2- Meshed polycrystals of geometry created using a Voronoi tessellation (a,b) and meshed bainitic microstructure obtained from a Voronoi tessellation and cell division to create laths (c).**

A real RPV steel microstructure is depicted in Fig. 3a using an inverse pole Figure map. As one can notice, the description used in Fig2c rely on metallurgical simplifications that could not be sufficient to capture the micro-structural complexity of mechanisms in RPV steel. A complementary approach to synthesis microstructures, of very versatile nature, is to use experimental 2D images to directly derive meshed microstructures from the images (this methodology will have to be extended to 3D situations). A result example is given in Fig. 3c created using the grain boundary image in Fig. 3b associated to the RPV microstructure in Fig. 3a.



**Figure 3- Image to mesh procedure of a real microstructure whose inverse pole figure map is given in (a) and grain boundaries in (b). The resulting mesh is shown on the right plot (c).**

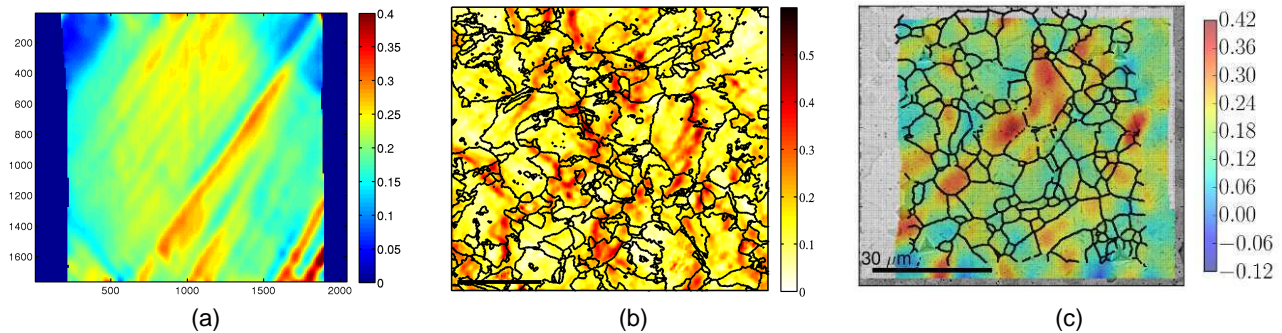
The meshed steel microstructures can then be used to perform Crystal Plasticity Finite Element Modelling (CPFEM) [9] which are the keystone to perform multi-scale studies of the plastic behaviour of steels. In the frame of the PERFORM European project [10], several crystal plasticity constitutive equations (e.g. [5]) have been implemented in the finite element code Code\_Aster. A result example of CPFEM calculation conducted with Code\_Aster on a pixel like microstructure derived from 2D EBSD data (as already introduced in [11]) is shown in Fig. 4, clearly highlighting strain localisation patterns occurring upon plastic deformation of the aggregate.



**Figure 4- Equivalent strain field calculated on the RPV steel microstructure with CPFEM Code\_Aster calculation.**

### 3. FIELD MEASUREMENTS : INTEGRATION OF THE KELKINS CODE AND SOME APPLICATION EXAMPLES

The digital image correlation (DIC) code KelKins [12] used to characterize strain localization phenomenon in steels as well as toughening mechanisms in nacre from in-situ atomic force microscopy pictures [13] has been implemented in the MAP platform. Initially developed in VisualC++ incompatible with linux environment and the MAP platform, the code has been improved to be easily compiled and used : a python wrapper calls C++ functions optimized for performance. Image outputs are created using the matplotlib package in python. In-situ SEM tensile experiments have been conducted on 304L stainless steel and a RPV sample prepared using a lithography grid patterning and chemical etching, respectively [14]. The DIC procedure allows to characterize strain localisation in a single grain of a 304L aggregate (Fig. 5a) or on a RPV steel aggregate (Fig. 5b) whose microstructure has been the support for the aforementioned studies (Fig. 3 and Fig. 4). Other in-situ experiments have also been conducted on Zircalloy-4 cladding materials (Fig. 5c) and future experiments will be conducted to study the effect of temperature on crystal plasticity behaviour for a wide range of steels.



**Figure 5 – Strain field measurements obtained by the DIC module in MAP on three different materials during in-situ SEM tensile experiments : 304L limited to a single grain (a), RPV steel polycrystal (b), and Zircalloy-4 polycrystal (c)**

Several procedures are being developed to take advantage of the spatially rich data, at the scale of the microstructure, that are obtained from in-situ experiment. One of the simplest approach has been presented in [14] and consists in combining local strain and crystal orientation data to estimate the plastic flow behaviour at the slip system scale. A second approach consists in performing finite element updating on a polycrystal CPFEM simulation [15] to identify the parameters of a crystal plasticity law : this activity is currently being conducted by A. Guery on a 316L material in collaboration with F. Hild and S. Roux at LMT Cachan and will be presented in a separate abstract.

### 4. PERSPECTIVES

We presented in this paper a limited number of key applications for which the MAP platform development is undertaken among other needs. During the conference, some additional applications in the field of microscopy imaging and calculation by homogenisation will also be presented. One global challenge is to bridge experiments and calculations, and having a platform where both experimental and calculated mechanical fields can be obtained will allow significant progress in this field. Although many achievements have been accomplished from 2D experimental and calculated data, additional difficulties are encountered for 3D situations, especially when one desire to generate model microstructures by meshing from experimental data available from diffraction contrast tomography [3] or automated 3D EBSD obtained by FIB erosion in a dual beam microscope. For this reason, in addition to developments conducted for meshing procedures, a promising direction of research is to use FFT [6] or Finite-Volume [16] elastic-viscoplastic calculations that show good performance for voxel-based microstructures.

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