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11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
E. Oñate, J. Oliver and A. Huerta (Eds)

IDENTIFICATION OF CRYSTAL PLASTICITY LAW PARAMETERS USING KINEMATIC MEASUREMENTS IN POLYCRYSTALS

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Key words: Crystal Plasticity, Identification, Digital Image Correlation

Abstract. From tensile tests on stainless steel specimen performed *in-situ* in a scanning electron microscope, displacement fields are measured using digital image correlation with an unstructured mesh taking as support the microstructure of the material. With this *same* mesh, finite element simulations are then performed using a crystal plasticity law and experimentally measured boundary conditions. The comparison of measured and simulated displacement fields leads to the identification of the sought parameters by resorting to a weighted finite element model updating method.

1 INTRODUCTION

The use of 316L(N) austenitic stainless steel in pressurized water reactor internals requires a good knowledge of its mechanical behavior. In particular, predictive constitutive models are established in micromechanical frameworks and take into account material ageing, for instance due to irradiation. Crystal plasticity models allow for accurate descriptions of intragranular plastic strains by considering the activity of slip systems [1]. However the identification of their constitutive parameters remains challenging [2]. In this paper, an identification procedure based on kinematic measurements in polycrystals during *in situ* tests performed in a Scanning Electron Microscope (SEM) is presented.

2 KINEMATIC MEASUREMENTS IN POLYCRYSTALS

To get experimental kinematic fields in polycrystals, a sequence of SEM images has been acquired during an *in situ* tensile test. A gray level texture is required with a dynamic range as large as possible with local contrast variations. In the present case, because the natural texture of the material does not provide such contrast, a computer-generated random pattern is deposited on the surface by lithography [3].

The displacement fields are measured between a reference image f and a deformed image g, with a continuous Galerkin based Digital Image Correlation (DIC) procedure [4, 5]. Thanks to electron backscattered diffraction acquisitions, the displacement discretization is performed using an unstructured mesh taking as support the grain boundaries (Figure 1), and composed of 3-noded triangular elements (about 20 pixel / 3 µm mean size). The size of the Region Of Interest (ROI) is 200 µm in width that corresponds to 1500 pixels. Image registration is performed by minimizing the quadratic norm of the difference between the reference image and the deformed image corrected by the displacement field. Namely, for a trial displacement field $\boldsymbol{v}$, the corrected deformed image, $\hat{g}(\boldsymbol{x}) = g(\boldsymbol{x} + \boldsymbol{v}(\boldsymbol{x}))$ can be computed, and the quadratic norm of the difference $\rho_c^2 = \|f - \hat{g}\|^2$ is minimized with respect to $\boldsymbol{v}$. In practice this minimization is performed by an algorithm where, at iteration n, the displacement field represented by a column vector of nodal displacement $\{\boldsymbol{u}^{(n)}\}$ is corrected by the increment $\{\boldsymbol{\delta u}^{(n)}\}$ solution of

$$[\boldsymbol{M}]\,\{\boldsymbol{\delta u}^{(n)}\} = \{\boldsymbol{b}^{(n)}\} \tag{1}$$

The matrix $[\boldsymbol{M}]$ and the vector $\{\boldsymbol{b}^{(n)}\}$ are known quantities, calculated from the gray levels f and g and the finite element shape functions $\boldsymbol{\psi}_k$ such that

$$M_{kl} = \sum_{ROI} (\boldsymbol{\psi}_k \cdot \nabla f)(\boldsymbol{x})(\boldsymbol{\psi}_l \cdot \nabla f)(\boldsymbol{x}) \tag{2}$$

and

$$b_k = \sum_{ROI} (f - \tilde{g}^{(n)})(\boldsymbol{x})(\boldsymbol{\psi}_k \cdot \nabla f)(\boldsymbol{x}) \tag{3}$$

where $\tilde{g}^{(n)}$ is the deformed image corrected by the current estimation of the displacement field. Because the noise of SEM imaging is relatively high (about 2% of the dynamic range of f) and the mesh fine, DIC calculations are assisted with mechanical regularization [5] with a regularization length equal to four times the characteristic length of the mesh.

Galerkin based DIC provides spatially dense kinematic measurements at the polycrystal scale (Figure 2(a) and 2(b)). This approach allows consistent comparisons to be performed with finite element calculations to identify material parameters by an inverse method.

3 SIMULATIONS OF EXPERIMENTAL TENSILE TESTS

Simulations of the experimental tensile test are performed using the finite element software Code_Aster and using a mesh built from that initially used for DIC. The resulting mesh is made of 4-noded tetrahedra created by extrusion with one element through the thickness for a 3D calculation. This direct link between DIC and simulations allows the experimentally measured boundary conditions with their time evolution to be prescribed without interpolation nor extrapolation.

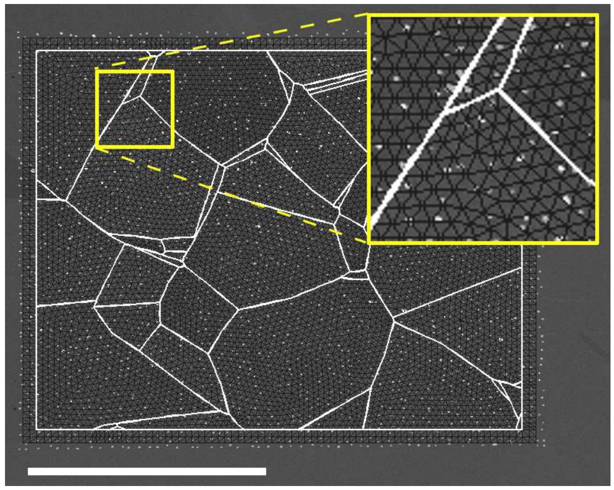


Figure 1: Unstructured mesh compatible with the underlying microstructure for DIC measurements. The scale bar is 100 μm

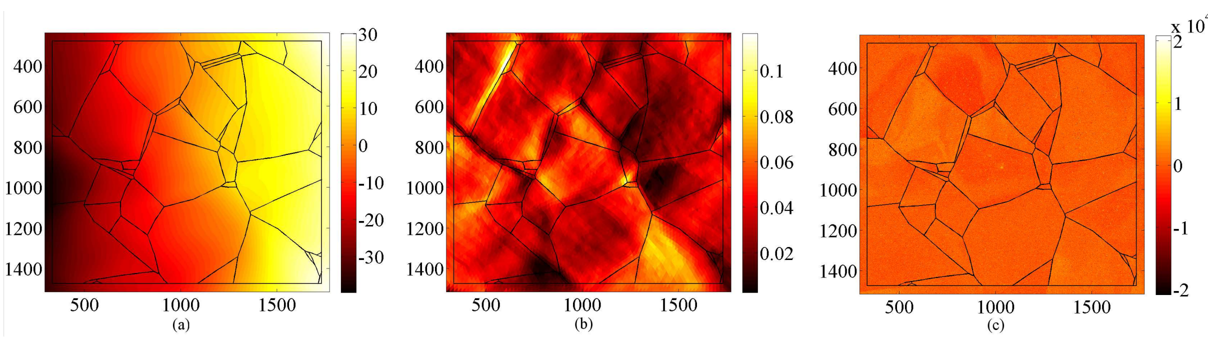


Figure 2: Displacement field expressed in pixels (a) and strain field (b) along the horizontal direction, measured experimentally for a macroscopic strain of 5%. The physical size of one pixel is 150 nm. Corresponding correlation residuals expressed in gray levels (c). The dynamic range of pictures is 16 bits. The grain boundaries are shown as black lines on these three fields

The crystal plasticity model chosen in this study has been proposed by Méric *et al.* in a study on the behavior of turbine blades under cyclic loadings [1]. It implies plastic flow (4, 5), isotropic (6) and kinematic (7) hardening relationships expressed for each of the 12 octahedral slip systems s:

$$\dot{\gamma}_s = \dot{p}_s \frac{\tau_s - c\alpha_s}{|\tau_s - c\alpha_s|} \tag{4}$$

$$\dot{p}_s = \left\langle \frac{|\tau_s - c\alpha_s| - R_s(p_s)}{k} \right\rangle^n \tag{5}$$

$$R_s = R_0 + q\left(\sum_{r=1}^{12} h_{sr}\left(1 - e^{-bp_r}\right)\right) \tag{6}$$

$$\dot{\alpha}_s = \dot{\gamma}_s - d\alpha_s \dot{p}_s \tag{7}$$

where c, k, n, R_0, q, b, d are constitutive parameters, and h_{sr} the coefficients of the interaction matrix between slip systems. The operator $\langle . \rangle$ takes the positive part of its argument. The three parameters associated with isotropic hardening are identified by homogenization [6] using the experimental macroscopic stress-strain data, the other parameters are set to previously identified values in case of cyclic loadings [7].

With this initial set of parameters, the simulated displacement fields are compared to the measured ones in Figure 3. The difference between these two fields at each time step is null at the edges of the ROI, since the experimentally measured boundary conditions are prescribed, and is to be minimized elsewhere in order to identify parameters of the crystal plasticity law.

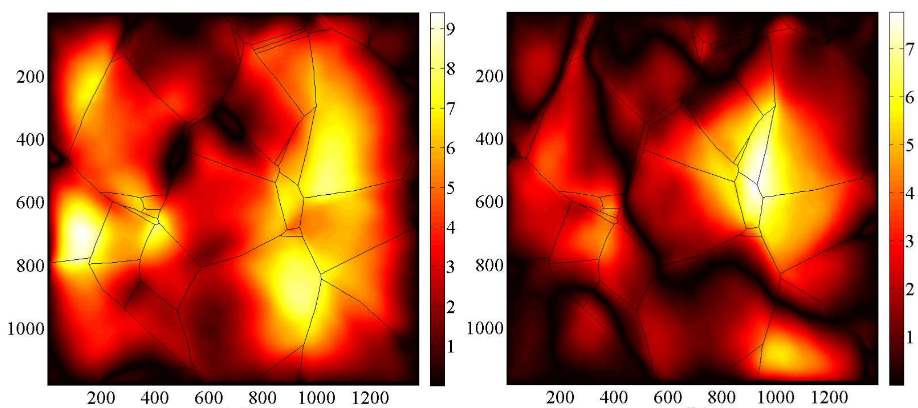


Figure 3: Absolute value of the difference between displacements fields expressed in pixels along the horizontal (a) and vertical (b) when measured by DIC and simulated by finite element computations for a macroscopic strain of 5 %. The set of parameters used for the simulation is that identified by homogeneization. The physical size of one pixel is 150 nm. The grain boundaries are shown as black lines on these three fields.

4 WEIGHTED FINITE ELEMENT MODEL UPDATING

To identify the three parameters associated with isotropic hardening, a weighted finite element model updating procedure is used. Such an inverse method has already been applied to J2-plasticity [8]. Specific developments have been proposed to regularize this ill-posed identification problem [9]. The cost function χ_T to be minimized is built from nodal in-plane displacements at each time step t, the load level and the measurement uncertainties. It is a combination of two contributions, one depending on the measured displacement fields, denoted χ_u, and the other one on the measured load level, denoted χ_F:

$$\chi_T^2(\boldsymbol{p}) = (1-w)\chi_u^2 + w\chi_F^2 \tag{8}$$

where w is a weight to be chosen between 0 and 1, χ_u^2 and χ_F^2 are expressed as:

$$\chi_T^2(\boldsymbol{p}) = (1-w)\frac{1}{2\eta_f^2 N_{dof} N_t}\sum_t \{\boldsymbol{\Delta u_t}\}^T [\boldsymbol{M}] \{\boldsymbol{\Delta u_t}\} + w\frac{1}{\eta_F^2 N_t}\{\boldsymbol{\Delta F}\}^T\{\boldsymbol{\Delta F}\} \tag{9}$$

where $\boldsymbol{p}$ is the set of parameters to identify, $\{\boldsymbol{\Delta u_t}\}$ the column vector of the difference evaluated at each degree of freedom between measured and simulated displacements at the time step t, $\{\boldsymbol{\Delta F}\}$ the column vector of the difference evaluated at each time step t between the experimental load and that obtained by a homogenization calculation [6] with the current value of $\boldsymbol{p}$. N_{dof} and N_t are respectively the number of degrees of freedom of the mesh and the number of time steps introduced to normalize $\{\boldsymbol{\Delta u_t}\}$ and $\{\boldsymbol{\Delta F}\}$. The DIC matrix $[\boldsymbol{M}]$ is used to weight the least squares criterion since it is related to the covariance matrix $[\boldsymbol{Cov_u}]$ of the measured kinematic degrees of freedom [10] for a given time step:

$$[\boldsymbol{Cov_u}] = 2\eta_f^2 [\boldsymbol{M}]^{-1} \tag{10}$$

where η_f is the standard deviation of noise of SEM images. The standard deviation of the load measurement, denoted η_F, is introduced to normalize χ_F. The minimization of χ_T is solved by successive linearizations and corrections.

Figure 4 shows the change of the cost functions χ_u and χ_F, of the load, and of the three parameters to be identified R_0, q and b, in a numerical test case. In that case a set of known values of parameters is to be identified (with no noise considered), with a starting gap of about 20 % of the reference values, and an equal weight for both cost functions (*i.e.*, $w = 0.5$). 22 iterations are required to identify the three parameters with an absolute error of 10^{-4}.

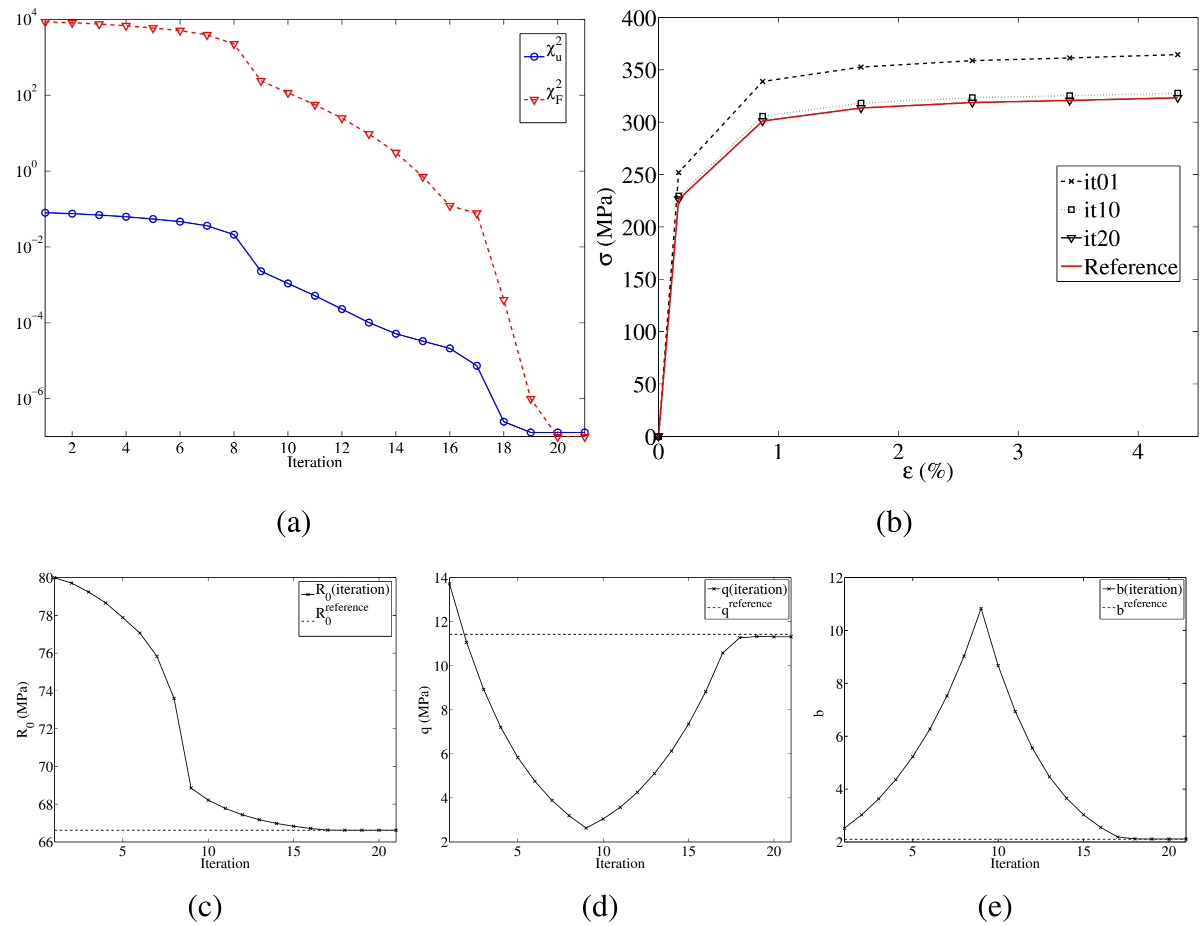
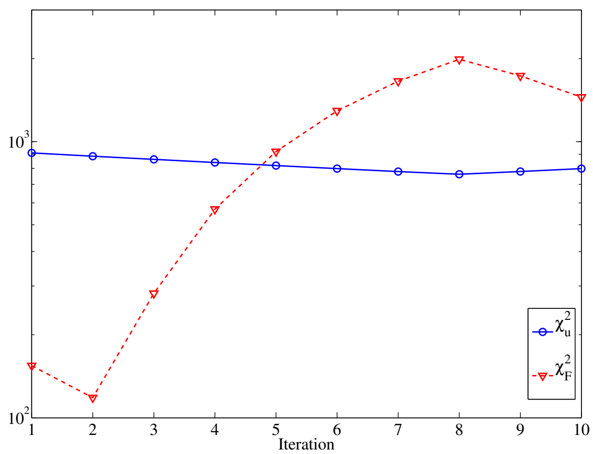
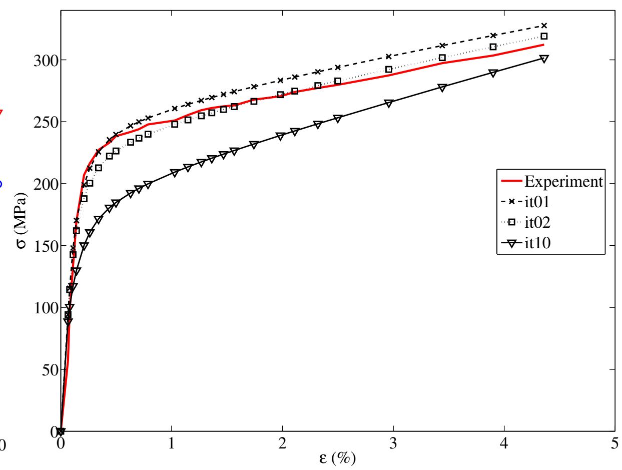


Figure 4: Numerical test case in which a set of reference values of the parameters is to be identified. Cost functions χ_u and χ_F as functions of the iteration of the identification procedure (a). Change of the macroscopic stress-strain curve wrt. iterations (b). Change of the parameters R_0 (c), q (d) and b (e), as functions of the iteration

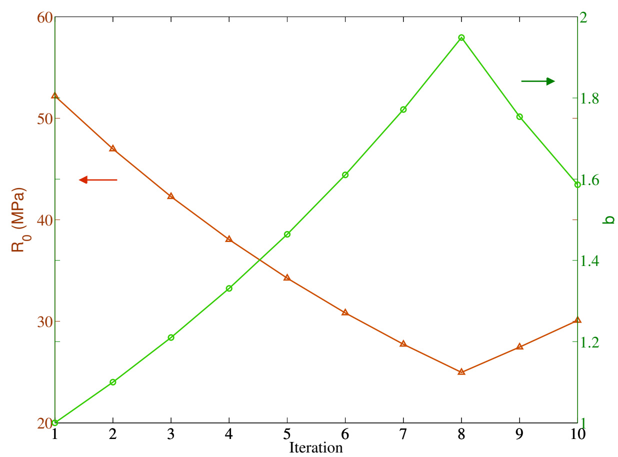
The identification in the experimental case is shown in Figure 5. The parameters R_0 and b are to be identified, starting from values identified by homogenization. The parameter q is chosen not to be identified but rather kept fixed, because as can be seen from Eq. 6 only the product qb comes into play for low values of p_r. In first trials, it was noticed that with an equal weight w (*i.e.*, $w = 0.5$), the identification procedure is led by the minimization of χ_F, which is equivalent to not considering displacement measurements. Therefore, a weight of 10^{-3} is chosen in order to favor the decrease of the displacements gap more than the global equilibrium gap. After 10 iterations, the levels of both cost functions remain high with respect to that of the noise (they would be unity if only noise is at stake in $\{\boldsymbol{\Delta u_t}\}$ or $\{\boldsymbol{\Delta F}\}$), and change slightly with more iterations. This high difference suggests a modeling error, that can be due to the microstructure not considered in the volume (because it was not experimentally characterised), due to the chosen boundary conditions, or even due to the chosen crystal plasticity law.



(a)



(b)



(c)

Figure 5: Analysis of the experimental case. Change of the cost functions χ_u and χ_F with the iteration of the identification procedure (a). Change of the macroscopic stress-strain curve with the iterations (b). Parameters R_0 and b as functions of the iteration number (c)

5 CONCLUSIONS

An identification procedure of parameters of a crystal plasticity model based on kinematic measurements in polycrystals of 316L(N) austenitic stainless steel has been presented. Displacement fields are measured on the surface of an *in-situ* tested specimen by digital image correlation using a mesh based on the actual crystallographic microstructure. A simulation of the same experiment is performed with an initial set of parameters. A weighted finite element model updating technique, using both displacement fields and load levels, is introduced. Results have been presented for a numerical test case to validate the numerical scheme, and for an experimental case. The identified values of the parameters depend of the relative weight given to the displacement fields or the load levels. The fact that the identification residuals are high is an indication that the assumed model is not fully consistent with the experimental observation. Other experiments with different grain sizes in the region of interest are being considered to assess the role of the microstructure on the identified parameters.

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