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1 **Identification methodology of a rate sensitive constitutive law with mean field and full**
2 **field modelling approaches for polycrystalline materials.**

3
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15
16 **Abstract:** the present paper deals with the consideration of the rate sensitivity mechanical
17 behavior of metallic materials, in the framework of mean field and full field homogenization
18 approaches. We re-examine the possibility of describing properly this rate sensitivity with a
19 simple and widely used power law expressed at the level of the slip system, and we propose a
20 methodology to accelerate the identification of the global material constitutive law for Finite
21 Element (FE) simulations. For such an aim, simulations of a tensile test are conducted, using a
22 simple homogenization model (the Taylor one, used in a relaxed constraint form) and a FE
23 code (Abaqus), both using the same single-crystal rate-dependent constitutive law. **It is shown**
24 **that, provided that the identification of this law is performed with care and well adapted to the**
25 **examined case (rate sensitive or insensitive materials, static and/or dynamic ranges), the**
26 **simple power law can be used to simulate the macroscopic behavior of polycrystalline**
27 **aggregates in a wide range of strain rate (including both static and dynamic regimes) and**
28 **strain rate sensitivity (up the rate-insensitive limit).**

29
30 **Keywords:** viscoplasticity, polycrystalline materials, strain-rate sensitivity, Finite Element.

31 1. Introduction

32

33 For the modelling of the global and local mechanical behaviors of polycrystalline metals in a
34 wide range of temperature or strain rate – with polycrystalline models, such as Taylor [1-3] or
35 Self Consistent models [4-6], with finite element (FE) codes [7-10], or with multiscale
36 approaches coupling DDD (Discrete Dynamic Dislocations) approaches with FE codes [11,
37 12] – it is quite usual to use a rate-dependent crystalline constitutive law, which generally
38 takes the form of the following power law expressed on the slip system s [1]^a

$$\dot{\gamma}^s = \dot{\gamma}_0^s \left(\frac{\tau^s}{\tau_0^s} \right)^n \quad (1)$$

39 In this expression, n (or more often $1/n = m$) characterizes the material rate sensitivity, $\dot{\gamma}^s$ is
40 the slip rate, and τ^s the resolved shear stress. The term τ_0^s is the so-called critical (or
41 reference) resolved shear stress (which evolves with strain when hardening is considered),
42 while the parameter $\dot{\gamma}_0^s$ is usually called a reference shear rate [7, 8, 12]. If the exponent n is
43 the same for all systems and for all grains of a polycrystal, it is easy to show that this
44 exponent is also the macroscopic rate sensitivity of the polycrystal as a whole [2]. By
45 assuming the rate dependence at the slip system level, this widely accepted phenomenological
46 law presents the double advantage of (i) assuming that plastic strain occurs solely by
47 crystallographic slip on well-defined slip systems, which is generally true for most metals at
48 not too high temperatures and (ii) suppressing the long standing problem of non-uniqueness in
49 the choice of active slip systems usually encountered in rate-independent crystalline plasticity
50 [13-15].

51 Such a viscoplastic crystalline law has also been shown to be able to provide physically
52 based large-strain rate-sensitive constitutive models, in order to interpret experiments on
53 metals performed up to quite large strain-rates (up to 10^4 s^{-1} , see e.g. [10]), in which
54 localization of plastic deformation is observed. Indeed, although rate sensitivity may be
55 neglected on purpose for many metallic alloys cold-deformed at low strain rates and strains,
56 this may no longer be valid when moderate or high strain rates are applied, or when high
57 temperature data are considered. It is now well-known that, in such a case, the resulting

^a By using only odd values of the exponent n , we avoid in the formulation the use of absolute values. Thus, the more classically chosen value of 20 will be replaced here by 21, **since the resulting difference in the macroscopic behaviour is hardly detectable.**

58 localization of plastic flow is indeed strongly influenced by the strain-rate sensitivity of the
59 material [16-18], and to a lesser extent by the deformation induced anisotropy [19]. Actually,
60 many authors have observed an increased rate sensitivity at large applied strain rates, and
61 have postulated that this rate sensitivity increase is a characteristic of the material [1, 10, 20,
62 21]. How large the strain rate must be to observe this increased rate sensitivity is still not
63 clear, however. Indeed, the strain rate sensitivity depends in quite a complex way on strain
64 rate, but also on strain, temperature, as well as on the underlying microstructure and possible
65 deformation mechanisms of the tested materials [6, 22-24]. Thus, a lot of successful
66 modelling efforts, some of them based on the very same power law as the one defined in
67 Eq. 1, have been made to be able to simulate different strain rate regimes, either controlled by
68 the thermally activated interactions between dislocations at rather low strain rates or by
69 dislocation drag at high strain rates (see, e.g. [25-28]). Conversely, some other authors claim
70 that accounting for rate sensitivity solely by a single relationship between shear rate and shear
71 stress is a too simplified approach even for low strain rates, and that this approach should be
72 replaced or completed by a rate-sensitive hardening law, describing the evolution of τ_0^S with
73 strain and strain-rate (e.g. [9, 29, 30]), to account for the right influence of strain-rate
74 sensitivity on the behavior of polycrystalline materials. Additionally, since this classical
75 power law is still mostly used with the aim of simplifying the numerical procedures by
76 providing a regularized form (with a unique solution on a given slip system) of the slip
77 criterion, the exponent n is usually not correctly set up (see below), resulting in an inaccurate
78 coupling between the macroscopic rate sensitive response and the rate sensitive evolutions of
79 critical resolved shear stresses of slip systems. In order to solve this problem **for rate-sensitive**
80 **or rate-insensitive materials**, some much more numerically efficient methods have been
81 recently proposed [29, 31]. **The first one [29] aims at describing properly the behavior of**
82 **materials in a wide range of rate-sensitivity and strain-rate, whereas the second one [31] aims**
83 **at being able to treat efficiently the case of rate-insensitive materials.** However, according to
84 the authors themselves, these efficient methods are not adapted either to the treatment of rate-
85 sensitive materials [31] or to their combined used with FE codes [32].

86 Thus, and especially in the framework of FE simulations, a lot of works are still based on
87 the use of the classical viscoplastic crystalline power law (Eq. 1), partly also rendered popular
88 by the UMAT (User Material) subroutine developed by Huang for the commercial software
89 Abaqus [33]. However, even in some very recent papers, the exponent of rate sensitivity is set
90 without any justification (e.g. [12]) or is *assumed* to be “adequately chosen to neglect the rate-

91 sensitivity” (e.g. [8, 16, 34]) at the polycrystal scale. In fact, it is easy to show that it is not the
92 case for many of the reported simulations, and that the choice made leads precisely to
93 unexpected high strain-rate sensitivity, as soon as the strain rate varies.

94 The aim of the present paper is thus to re-address the question, **and the use**, of the applied
95 strain-rate sensitivity in computations using a power law based crystal plasticity model, **for**
96 **both rate-insensitive and rate-sensitive materials**. We will first **recall the procedure to use**
97 **adequately such a simple formulation for rate-insensitive materials**. With the addition of
98 the phenomenological saturating hardening law used in [33], we will then **propose a**
99 **methodology to accelerate the identification of the parameters describing the**
100 **constitutive law of the material, with a FE code, for rate-sensitive materials at rather low**
101 **strain rates (i.e. within the static regime). We will finally show that this identification can**
102 **be extended to the case of high strain rates (dynamic regime), provided that the n value**
103 **is identified differently in both regimes**. This will be illustrated by some simulations of a
104 tensile test performed using two different modelling approaches, i.e. a simple homogenization
105 model (the Taylor one, used in a relaxed constraint form) and a FE computation (using
106 Abaqus software and dedicated User Subroutines [33]), both approaches using the very same
107 single-crystal rate-dependent constitutive law and allowing strain rate fluctuations within the
108 polycrystalline material.

109 The outline of the present paper is thus the following: the classical single crystal
110 viscoplastic flow rule and associated hardening law are presented in **Section 2**, its
111 implementation into the Taylor model and FE Abaqus code are briefly described in **Sections 3**
112 **and 4**, the results of the performed simulations are then analyzed in **Section 5** and some
113 conclusions are drawn in **Section 6**.

114

115 **2. The classical single crystal viscoplastic flow rule and associated hardening law**

116

117 As already mentioned, when a grain g of a polycrystalline sample is subjected to a stress state
118 $\boldsymbol{\sigma}$, plastic strain takes place by slip on several slip systems, each labeled by index s . At the
119 level of the slip systems, the rate dependent slip criterion is given by Eq. 1. The resolved
120 shear stress on system s is equal to $\tau^s = \sigma_{ij}R_{ij}^s = S_{ij}R_{ij}^s$, \mathbf{S} being the (symmetrical) deviatoric

121 stress tensor and \mathbf{R}^s the orientation tensor of system s^b . The components of this last tensor
 122 read

$$R_{ij}^s = \frac{1}{2}(n_i^s b_i^s + b_i^s n_i^s) \quad (2)$$

123 with \vec{n}_s and \vec{b}_s characterizing respectively the slip plane normal and the slip direction for the
 124 system s . The strain rate tensor $\dot{\boldsymbol{\varepsilon}}$ in grain g is then defined as a summation of individual
 125 shear-rate components on all systems s :

$$\dot{\varepsilon}_{ij} = \sum_s \dot{\gamma}_0^s \left(\frac{\tau^s}{\tau_0^s}\right)^n R_{ij}^s = \sum_s \dot{\gamma}_0^s \left(\frac{S_{kl} R_{kl}^s}{\tau_0^s}\right)^n R_{ij}^s \quad (3)$$

126 As long as the parameters τ_0^s , $\dot{\gamma}_0^s$ and the exponent of rate sensitivity n are constant, this
 127 equation represents a unique relationship between strain rate and deviatoric stress tensors at
 128 the level of grain g , which allows to determine both tensors from the boundary conditions
 129 imposed to the considered grain (more precisely 5 independent components for each tensor).
 130 The existence of a unique solution has the direct consequence that the current stress state vary
 131 with strain rate and vice versa. This constitutive law is classically accompanied by a
 132 hardening law, which can be expressed – again at the level of the slip systems – as

$$\dot{\tau}_0^s = \sum_l H_{sl} \dot{\gamma}^l \quad (4)$$

133 with H_{sl} the components of the so-called hardening matrix. As in the UMAT subroutine
 134 developed for Abaqus, a saturating expression – which has proven its efficiency to reproduce
 135 experimental data concerning several metallic alloys [35, 36] – can be adopted which reads

$$\begin{cases} H_{ss} = h_0 \operatorname{sech}^2 \left| \frac{h_0 \bar{\gamma}}{\tau_{sat} - \tau_{ini}} \right| \\ H_{sl, s \neq l} = q h_0 \operatorname{sech}^2 \left| \frac{h_0 \bar{\gamma}}{\tau_{sat} - \tau_{ini}} \right| \end{cases} \quad (5)$$

136 where $\bar{\gamma}$ is the cumulated shear strain on system s so that

^b In the following, tensors are written in bold, and the subscript ‘M’ denotes macroscopic values.

$$\bar{\gamma} = \int_0^t \sum_s |\dot{\gamma}^s| dt \quad (6)$$

137 In order to characterize completely these laws (Eqs. 5 and 3), 4 material parameters are thus
 138 needed, namely τ_{ini} , τ_{sat} , q and h_0 , together with two other sets of material parameters, τ_{0ini}^s
 139 (initial values) and $\dot{\gamma}_0^s$ – which can be reduced to 2 parameters τ_{0ini} and $\dot{\gamma}_0$ if they are
 140 assumed equal for all systems in all grains – and finally the exponent of rate sensitivity n . If
 141 one single value τ_{0ini} is imposed for all systems, then it is trivial to set it equal to τ_{ini} . In that
 142 case, the τ_{ini} and τ_{sat} values are directed linked to the initial and final values of both
 143 microscopic (at the level of the grain) and macroscopic stress values (see Figure 1 below). As
 144 for the h_0 hardening coefficient, it affects the hardening rate all along the stress – strain curve
 145 before the saturation level is reached (see again Figure 1).

146 Now, in order to demonstrate the usefulness of the proposed crystalline law, we are going
 147 to use two different simulations approaches (i.e., mean and full field ones) to calculate the
 148 macroscopic response of a polycrystalline aggregate in uniaxial tension; for both approaches,
 149 by construction, the local strain rate is allowed to differ from one grain to another and thus
 150 may be quite different from the macroscopic imposed one.

151

152 3. Simulation framework

153

154 3.1 The Taylor model (with full or relaxed constraints)

155 In the framework of the Taylor model (FC – Full Constraint or RC – Relaxed Constraint),
 156 several options are possible to simulate a tensile test along, e.g., the axis 3 of the macroscopic
 157 reference system:

- 158 (i) the Taylor model in the FC mode, which implies that all components of the strain rate
 159 tensor within each grain are assumed to be the same than the imposed macroscopic
 160 ones, i.e. $\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{E}}_M$. For a general anisotropic material, the combined boundary
 161 conditions in terms of stress and strain rate then read at the level of the grain

$$\dot{\boldsymbol{\epsilon}} = \dot{E}_{33imp} \begin{vmatrix} -\alpha & 0 & 0 \\ 0 & 1 - \alpha & 0 \\ 0 & 0 & 1 \end{vmatrix} \quad \text{and} \quad \boldsymbol{\sigma} = \begin{vmatrix} 0 & ? & ? \\ ? & 0 & ? \\ ? & ? & ? \end{vmatrix} \quad (7)$$

162 in which \dot{E}_{33imp} is the imposed macroscopic strain rate along the tensile axis and α the
 163 so-called contraction ratio, which has to be calculated, for each calculation step, by

164 minimizing the macroscopic plastic work rate with respect to α [37]. If the material is
 165 isotropic, this factor is set to be equal to 0.5 and no extra minimization procedure is
 166 necessary in this case. **This case is known to represent an upper bound for the**
 167 **macroscopic behavior of the material.**

168 (ii) the Taylor model in its most relaxed version, often called the Sachs–Köcherdorfer
 169 model [38, 39]. In this case, a uniaxial stress state is applied to each grain, and only the
 170 macroscopic strain rate along the tensile axis \dot{E}_{33} is imposed in each grain. The
 171 boundary conditions are then

$$\dot{\boldsymbol{\varepsilon}} = \dot{E}_{33} \text{imp} \begin{vmatrix} ? & ? & ? \\ ? & ? & ? \\ ? & ? & 1 \end{vmatrix} \quad \text{and} \quad \boldsymbol{\sigma} = \begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & ? \end{vmatrix} \quad (8)$$

172 This option is usually applied for small strains, but it is considered to be far from the
 173 reality for moderate or large ones. **It is worth mentioning that, as one of the**
 174 **5 independent components of the strain-rate tensor is still imposed to each grain, this**
 175 **model does not corresponds to the so-called static model which constitutes the lower**
 176 **bound for the macroscopic behavior and for which the total stress tensor is the same for**
 177 **all grains.**

178 (iii) an “intermediate” approach (**which will be called RC – Relaxed Constraints – Taylor**
 179 **model in the following**), which is thought to be better for anisotropic materials although
 180 quite simplified, which consists in allowing the contraction ratio α to be different within
 181 each grain, which implies the following boundary conditions

$$\dot{\boldsymbol{\varepsilon}} = \dot{E}_{33} \text{imp} \begin{vmatrix} ? & 0 & 0 \\ 0 & ? & 0 \\ 0 & 0 & 1 \end{vmatrix} \quad \text{and} \quad \boldsymbol{\sigma} = \begin{vmatrix} 0 & ? & 0 \\ ? & 0 & ? \\ ? & ? & ? \end{vmatrix} \quad (9)$$

182 It is easy to prove that, if the sample is isotropic, we will get $\dot{E}_{M22} = \dot{E}_{M11} = 0.5$ at the
 183 level of the polycrystal and the resulting macroscopic stress state will also be purely
 184 uniaxial (like in the FC mode). Apart from being simpler and more rapid than the FC
 185 one, this version is thought to be especially well adapted to the simulation of a tensile
 186 test applied on anisotropic materials (as well as in isotropic ones of course) [40], and is
 187 consequent used in the present work.

188 For all these cases, it is readily seen that, among the 10 independent components of $\dot{\boldsymbol{\varepsilon}}$ and $\boldsymbol{\sigma}$
 189 which need to be determined, 5 are imposed and the 5 remaining are deduced from Eq. 3. The
 190 associated macroscopic quantities $\dot{\boldsymbol{E}}_M$ and $\boldsymbol{\Sigma}_M$ are then obtained by averaging on all grains.

191 Once the boundary conditions have been selected, an iterative calculation can be

192 performed to simulate a tensile test, and, from the boundary conditions expressed by Eq. 9
 193 and the resolution of Eq. 3, the tensile deviatoric stress S_{33} and strain rate $\dot{\epsilon}_{33} = \dot{E}_{33imp}$ can
 194 be extracted at each step of the calculation (characterized by a time increment Δt). Then, at a
 195 given time t of the simulation, the total tensile strain can be obtained:

$$\Delta E_{33} = \dot{E}_{33imp} \Delta t \Rightarrow E_{33}(t + \Delta t) = E_{33}(t) + \dot{E}_{33imp} \Delta t \quad (10)$$

196 At each step, the reference shear stress of each system, within each grain, is also updated

$$\tau_0^s(t + \Delta t) = \tau_0^s(t) + \sum_l H_{sl} \dot{\gamma}^l(t) \Delta t \quad (11)$$

197 noting that, at time $t=0$, $\tau_0^s = \tau_{ini}$ and $\sum_l H_{sl} \dot{\gamma}^l(t) = 0$.

198 In order to calculate the macroscopic tensile curve, the deviatoric stress is averaged on all
 199 grains at each step to get S_M and the macroscopic true tensile stress Σ_{M33} . As

$$S_{Mii} = \langle S_{ii} \rangle \quad \text{and} \quad \Sigma_{Mii} = S_{Mii} + \frac{P}{3} \quad (12)$$

200 where P is the hydrostatic pressure, and since the macroscopic boundary conditions also
 201 impose that

$$\Sigma_{M11} = \Sigma_{M22} = 0 \quad (13)$$

202 then, we simply get

$$\Sigma_{M33} = \frac{3}{2} S_{M33} \quad (14)$$

203 Eqs. (10) and (14) allow then to plot the macroscopic tensile stress – strain curve. Since
 204 \dot{E}_{33imp} is imposed and constant along the test, the final strain can be written as

$$E_{33final} = \dot{E}_{33imp} N_{step} \Delta t \quad (15)$$

205 with N_{step} the total number of calculated steps. It is thus readily seen that if \dot{E}_{33imp} is
 206 modified, the product $N_{step} \Delta t$ has to be modified as well to keep the first term of Eq. 15
 207 constant. In many of the papers quoted above which deal with the influence of strain rate
 208 sensitivity, the macroscopic strain rate is rarely varied and only the influence of the exponent
 209 n is studied: it is for example mentioned by Canova and co-workers [1] that “all the results
 210 are normalized by the Von Mises (VM) equivalent strain-rate and are thus independent of the
 211 applied strain rate”. In the present case, the grain VM equivalent strain rate indeed varies from
 212 grain to grain, for the selected boundary conditions (it would not be the case of course for the

213 FC assumption). The same expression is also valid at the macroscopic level, but if the
214 material is macroscopically isotropic, it simply becomes equal to

$$\dot{E}_{VM} = \dot{E}_{33imp} \quad (16)$$

215 In the simulations performed below, we will thus have $\dot{\epsilon}_{VM} \neq \dot{E}_{VM}$ in most of the grains.
216 Also, as in many publications listed above, using either an homogenization model or a FE
217 code, a reference case will be defined as the one performed by defining the reference shear
218 rate equal to the macroscopic one, that is $\dot{\gamma}_0 = \dot{E}_{33imp}$, which means $\dot{E}_{33imp}/\dot{\gamma}_0 = \dot{E}_{VM}/\dot{\gamma}_0 =$
219 1. As a consequence, if the macroscopic strain rate \dot{E}_{VM} is multiplied or divided by a factor of
220 say 10, without modifying the value of the reference shear rate $\dot{\gamma}_0$, N_{step} will have to be
221 divided or multiplied by 10, if $E_{33final}$ and Δt are kept constant. The exponent n will be
222 varied in a wide range associated classically with room temperature deformation, i.e. between
223 10 and 200. This model will be used below to reproduce the mechanical behavior of several
224 FCC materials (stainless steel and aluminum alloy) extracted from the literature. As in the
225 selected examples, the texture is not documented or assumed to be isotropic, it is considered
226 in the following only isotropic aggregates, represented by a set of 2016 orientations,
227 uniformly distributed within the Euler space. For all treated examples, the 12 $111\langle 110 \rangle$
228 systems will be considered. It is worth to point out that the aim of the present work is not to
229 demonstrate the relevance of the RC Taylor model, but to be able to study the influence of the
230 simple rate-sensitivity power law in a model allowing a strain rate gradient within the
231 aggregate. Some tensile curves have been simulated with this approach to illustrate the
232 influence of the various hardening parameters on the global response. These are shown in
233 Figure 1, where it can be clearly seen that, for a given modelling approach, the initial value
234 (resp. final value) of the macroscopic tensile stress is directly proportional to the value of
235 $\tau_0 = \tau_{ini}$ (resp. τ_{sat}). This proportionality is even independent of the selected hardening law
236 for the yield stress value.

237

238 **3.2 The FE Abaqus code**

239 As the objective is to deal with strain-rate sensitivity in the framework of FE codes, some
240 simulations have also been performed with the FE code Abaqus, which is increasingly used
241 for the simulation of the VP behavior of polycrystalline materials, with the very same
242 description of the single crystal constitutive law. Again isotropic materials are considered. The
243 simulation of a tensile test with such a code, however, is usually not performed with exactly

244 the same boundary conditions as the ones imposed in the RC Taylor model, since
245 displacements, instead of strain rates, are generally applied in FE simulations. Furthermore,
246 the description of the initial microstructure of the material is also somewhat different, since it
247 accounts for both orientations and positions of the grains within polycrystalline aggregates,
248 whereas only the orientation distribution is accounted for in the Taylor model.

249 In the present case, the considered isotropic material will be represented by a cubic
250 polycrystalline aggregate of 200 grains, made of a Voronoï tessellation obtained from Neper
251 program [41] and imported in Abaqus CAE using python scripts [42] (see Figure 2a). The
252 grain boundaries are simply defined as the boundaries between zones of different orientations.
253 The choice of a reduced number of orientations compared to the previous case appears here to
254 be a good compromise to obtain both reasonable calculation times and a macroscopic uniaxial
255 tensile stress, as with the **RC Taylor** model. The polycrystal is submitted to both symmetry
256 boundary conditions and imposed displacement on the upper and lower faces, while on the
257 lateral ones, uniform mixed-orthogonal (or block) conditions have been defined to account for
258 periodicity [43, 44] (Figure 2b).

259 The crystal plasticity mechanical behavior, as defined in Eqs. 1 to 6, is introduced into Abaqus
260 using a UMAT subroutine, which is extensively described in [33], and the Euler angle set
261 $(\varphi_1, \Phi, \varphi_2)$ of each Voronoi cell is randomly determined in an ORIENT subroutine, describing
262 thus an isotropic angle set.

263

264 **4. Numerical results**

265 ***4.1 Case study 1: the case of a rate-insensitive material***

266 The first example treated with the simple RS constitutive law described above is the often
267 encountered case of a material with a very low strain-rate sensitivity (represented by $1/n$).
268 This in turns means a very high value of the n exponent. This exponent is usually established
269 experimentally from flow stresses obtained at different strain rates but same microstructural
270 state (e.g., dislocation density and thus same stress level), from the slope of the ln–ln stress–
271 strain rate curve [45]:

$$n = \left. \frac{\partial \ln \dot{E}_M}{\partial \ln \Sigma} \right|_{\Sigma} \quad (17)$$

272 When doing so, values as high as 100–400 have been reported in the literature for various
273 materials (copper, brass, many steels,) and this is why some regularized versions of the

274 present VP formulation have been proposed since calculations performed with very high
275 values of n (above 200) are practically impossible to achieve, whatever the model used [29,
276 31]. Another way of solving this problem is to embed the norm of the applied strain rate into
277 the reference shear rate $\dot{\gamma}_0^s$ [30], by imposing it to be equal to the applied macroscopic strain
278 rate, i.e. $\dot{\gamma}_0^s = \dot{E}_{33imp}$ in the present case. It is then easy to show that in this case, the
279 macroscopic response does not depend on the selected n value, and that the magnitude of the
280 grain stress is affected only by the ratio of the grain strain rate magnitude and the macroscopic
281 strain rate magnitude, which is not so large for FCC materials. This procedure is frequently
282 used, especially when simulations are performed for one single macroscopic strain rate value.

283 Let us reproduce in this way, an experimental curve obtained at room temperature for a
284 304L stainless steel, whose texture is assumed to be isotropic [46]. In order to identify the
285 hardening parameters for this case, the reference shear stress has been set equal to the actual
286 strain rate, i.e., 0.001 s^{-1} , and the n exponent to 21, i.e. one of the value most often found in
287 the literature “to reproduce negligible viscous behavior” [47] or for material which “possesses
288 a certain rate-dependency at medium to high temperatures” [14, 34, 48-51]. The other
289 material parameters have been manually identified on the experimental curve (see Figure 3);
290 they are listed in Table I.

291 It is seen that, for the selected parameters, the agreement, although not 100% perfect, is
292 quite satisfactory. An automatic identification procedure or the selection of a more physically-
293 based hardening law would probably allow for a better fit over the whole strain range, but this
294 is out of the scope of the present paper. Much more important, for it is the focus of the present
295 study, it is seen that when $\dot{\gamma}_0 = \dot{E}_{VM}$, the influence of the exponent n is indeed very limited
296 and negligible for $n \geq 21$, as reported in many studies using the same law.

297 But, once this reference case is satisfactorily treated, we may want to see what would
298 happen if we change now the applied strain rate without changing the value of the reference
299 shear stress $\dot{\gamma}_0$. This is illustrated in Figure 4, where simulations have been made using the
300 parameters listed in Table 1, except for the applied normalized strain rate $\dot{E}_{VM}/\dot{\gamma}_0$ which has
301 multiplied or divided by ten and the exponent n which has been varied from 21 to 111. It is
302 seen that, when the normalized strain rate is set to $\dot{E}_{VM}/\dot{\gamma}_0 = 1/10$, there is an influence of
303 the strain rate on the macroscopic response, and that the curves are almost superimposed only
304 for $n \geq 91$. It is interesting to note that the best agreement with the experimental curve is
305 now found for $n = 41$, which means that both reference strain rate $\dot{\gamma}_0$ and exponent n should

306 be considered simultaneously for the identification of the hardening parameters, as done in
307 other works, see e.g. [9]: for the identification of the selected 304L tensile curve, taking
308 $\dot{\gamma}_0 = 10 \times \dot{E}_{VM}$ with $n = 41$ indeed provides a slightly better fit than $\dot{\gamma}_0 = \dot{E}_{VM}$ with
309 $n = 21$. It is also seen in Figure 4a that the overall stress level is increasing with n , when
310 $\dot{E}_{VM} < \dot{\gamma}_0$, as a consequence of the used power law.

311 If the normalized strain rate is set to $\dot{E}_{VM}/\dot{\gamma}_0 = 10$, there is again a clear influence of the
312 strain rate on the macroscopic response, and the curves are again almost superimposed only
313 for $n \geq 91$. The overall stress level is now decreasing when n increases, which better
314 correspond to the expected influence of rate sensitivity and has already been observed in some
315 other works: for example, these calculations are in full agreement with the ones performed by
316 Khan et al. [9] with a similar power law.

317 Some curves obtained for two different values of n , namely 21 and 111 and various
318 values of $\dot{E}_{33imp}/\dot{\gamma}_0$ between 1 and 10^{-4} (that is 4 orders of magnitude) are now presented in
319 Figure 5. These curves have been obtained with the RC Taylor model as well as with Abaqus,
320 with the same material parameters. For the FE simulation, as the elastic part of the curve is
321 also simulated, the following elastic constants have been considered for 304L steel:
322 $C_{11}=197500$ MPa, $C_{22}=125000$ MPa and $C_{44}=122000$ MPa. As the boundary conditions
323 imposed to simulate a simple tensile test are not exactly expressed in the same way for the
324 two approaches, before performing comparisons of the two sets of calculations, it has been
325 checked that the macroscopic tensile test was indeed uniaxial in both cases (this would not
326 have been necessarily the case for an anisotropic material). For comparison purposes, the
327 elastic part of the curves has been taken out from the Abaqus simulations. It is interesting to
328 note that the Abaqus curves are systematically below the RC Taylor curves, even though the
329 Taylor model is not used in the pure FC mode (which would actually correspond to an upper
330 bound). This means that the interactions between grains are softer in Abaqus than with the
331 selected RC Taylor model. However, it is clear that the influence of the strain rate for given
332 values of $\dot{\gamma}_0$ and n are similar for both approaches. It is also worth noting that $n \geq 111$, the
333 convergence is very difficult to achieve with Abaqus, depending on the material description
334 and imposed strain rate.

335 The influence of the normalized strain rate $\dot{E}_{VM}/\dot{\gamma}_0$ and strain rate sensitivity exponent
336 n on the overall yield stress is now presented in Figure 6 for all performed situations. This
337 yield stress is extracted at the first calculation step for the RC Taylor simulations and

338 evaluated at 0.02% plastic strain for the Abaqus simulations. Clearly this stress value does not
339 vary much with the exponent for $\dot{E}_{VM}/\dot{\gamma}_0 = 1$ in both cases, but when this value is changed,
340 the stress can strongly vary: for example, for $n=21$, the stress varies from about 180 to
341 310 MPa when $\dot{E}_{VM}/\dot{\gamma}_0$ varies from 0.0001 to 10 with the RC Taylor model; similarly, with
342 Abaqus, the stress varies from 170 to about 263 MPa when $\dot{E}_{VM}/\dot{\gamma}_0$ varies from 0.0001 to 1.
343 The response of the material is thus clearly rate-sensitive for $n=21$. The absence of strict
344 linearity observed in the Abaqus simulations can be attributed to numerical reasons and to the
345 local fluctuations of strain rate and stress, more significant than with the RC Taylor model,
346 associated with weaker interactions between grains.

347 Now, by calculating the normalized ratio of this tensile yield stress by the reference shear
348 stress (taken here equal to 100 MPa), the RC Taylor and Abaqus responses can be compared
349 to the Upper and Lower Bounds rate-insensitive approaches. It is indeed well known that, for
350 an isotropic FCC metal in the rate-insensitive limit, this normalized stress is equal to 3.06 for
351 the upper bound (Taylor model), 2 for the lower bound (static model) and 2.2 for the Sachs –
352 Kochendorfer model [52]. It is also clear from Figure 6, that this rate-insensitive value can be
353 estimated for the viscoplastic RC Taylor and Abaqus models from the yield stress obtained for
354 $\dot{E}_{VM} = \dot{\gamma}_0$ and the highest possible value for the exponent n . The so-obtained values are 2.78
355 for the RC Taylor model and about 2.62 for Abaqus. This confirms that the RC Taylor
356 approximation is closer to the upper bound than to the lower one and that the interactions
357 between grains are slightly softer with Abaqus. This also affects the hardening capacity as
358 seen in Figure 5.

359 This first study has highlighted the fact that the only way to really neglect rate sensitivity with
360 the power law is to set $\dot{\gamma}_0 = \dot{E}_{VM}$ and to keep the macroscopic strain rate constant; this is
361 indeed well known from experienced users of VP mean field or full field methods, but much
362 less from new FE codes users, if we look at the recent bibliography on the subject.

363

364 ***4.2 Case study 2: the case of a rate-sensitive material***

365 Furthermore, if some alternatives exist to treat efficiently the case of the rate-insensitive
366 materials, the simple power law (Eq. 1) is still largely used to treat the case of rate-sensitive
367 materials **within the static regime (typically for strain rates staying below 1.0 s^{-1})**. Of course,
368 as already said, it cannot alone account for the complex rate-sensitivity influence of a real
369 material and the rate sensitivity of the hardening rate should also be considered [9, 32],
370 especially if the treated problems involve strong flow localization [53, 54]. But, if it is not the

371 case, i.e. for moderate strains and strain rates, Christodoulou and Jonas [54] have shown that
372 the use of the so-called continuous strain-rate sensitivity as defined by Eq. 17, i.e. determined
373 at constant structural state, instead of a more instantaneous one, determined during strain rate
374 change tests, compensates to some extent for the neglect of the rate sensitivity of hardening.
375 Thus, even with a rather simple hardening law, by paying attention to the identification
376 procedure, it can still reproduce quite precisely the observed behavior of materials tested at
377 different strain rates and be useful for simulations for which strong localization is not
378 expected. Let us take the example of pure aluminum (99.99%), which is more rate sensitive
379 than the previously studied steel. Some experimental data have been extracted from [53, 54]
380 and the rate sensitivity of the material has been estimated using Eq. 17 (Figure 7). The
381 resulting estimated n value is found to be equal to 15 for an explored strain-rate range of 0.05
382 to 0.0005 s^{-1} .

383 Then, as in the previous example, the identification of the hardening parameters have
384 been made for a reference case, corresponding to $\dot{\gamma}_0 = \dot{E}_{VM}$, arbitrarily selected equal to
385 0.0005 s^{-1} . We have also fixed the value of q to 1.1, classically selected for aluminum.
386 Therefore, 3 parameters remain to be determined, which are $h_0, \tau_{ini}, \tau_{sat}$. These 3 parameters
387 have been manually adjusted to reproduce the curve corresponding to $\dot{E}_{VM} = 0.0005 \text{ s}^{-1}$ and
388 validated then by simulating the other curves corresponding to $\dot{E}_{VM} = 0.005 \text{ s}^{-1}$ and
389 $\dot{E}_{VM} = 0.05 \text{ s}^{-1}$. The result of this first identification is presented in Table II and Figure 8a,
390 in which the elastic parts of the experimental curves have been suppressed. In the validation
391 process, the parameters may be slightly re-adjusted. In that case, they have to be validated
392 again on the reference case.

393 Once the parameters have been selected for the whole explored strain-rate range, it may
394 be desirable to modify the reference case, and thus the value of the associated reference
395 strain-rate $\dot{\gamma}_0$. In that case, it is not necessary to perform the whole identification and
396 validation process; it can simply be noticed that for a given model, the results of a 2nd
397 identification procedure should coincide with the result of the 1st one, since the curves to be
398 identified are precisely the same. In other words, if the material parameters are changed, the
399 predicted stress and strain-rate tensors at the level of the grains as well as at the level of the
400 sample should coincide at each step of the calculation and especially at the very beginning
401 and at the saturation level (although this level may be not reached experimentally). From Eq.
402 3 and the definition of τ_{ini} and τ_{sat} , this implies that

$$\frac{\dot{\gamma}_0}{\tau_{ini}^n} = constant \quad \text{and} \quad \frac{\dot{\gamma}_0}{\tau_{sat}^n} = constant \quad (18)$$

403 from which the new values of τ_{ini} and τ_{sat} associated with the new selected value of $\dot{\gamma}_0$ can
 404 be extracted. There remains then one single parameter to be identified, namely the hardening
 405 coefficient h_0 . The results of this procedure applied to the new reference case $\dot{\gamma}_0 = \dot{E}_{VM} =$
 406 0.05 s^{-1} are also presented in Table 2 and Figure 8b. It is seen that the identified curves are
 407 very close to the ones obtained previously for the other set of parameters. Of course, for such
 408 a simple model, simulations are quite rapid (typically less than one minute for the calculation
 409 of one single curve in the presented examples), and thus the total identification procedure,
 410 whether performed manually as in the present case, or through an optimized identification
 411 procedure is also quite fast.

412 Contrary, for FE simulations, the identification of one set of parameters on one reference
 413 curve and the validation on the other two would take much longer times (depending on the
 414 computer). We can however accelerate the procedure if we first base our identification
 415 procedure for FE simulations on a preliminary identification step performed with a simpler
 416 model like the Taylor one as explained below.

417 In order to perform the identification of the 3 presented Al curves with Abaqus, it is first
 418 set again $n = 15$ and $q = 1.1$. The following elastic constants are also considered for
 419 aluminum: $C_{11}=108240 \text{ MPa}$, $C_{12}=62 \text{ 160 MPa}$ and $C_{44}=28410 \text{ MPa}$. Then one reference case is
 420 selected, for example the same as previously, $\dot{\gamma}_0 = \dot{E}_{VM} = 0.0005 \text{ s}^{-1}$ and a first calculation
 421 is performed with Abaqus (*sim1*) **with the 3 hardening parameters issued from the RC**
 422 **Taylor identification**, called in the present case h_{01} , τ_{ini1} , τ_{sat1} . As the two approaches do
 423 not lead to the same response (see Figure 5), it is expected that the predicted curve will not
 424 perfectly fit the experimental one. One first correction can be made on τ_{ini} by using the
 425 proportionality relationship between initial stress σ_0 and τ_{ini} , illustrated in Figure 1, i.e.:

$$\frac{\sigma_{0sim1}}{\tau_{ini1}} = \frac{\sigma_{0exp}}{\tau_{ini}} \cong \frac{\sigma_{0Tay}}{\tau_{ini}} \quad (19)$$

426 In this expression, σ_{0Tay} represents the value of the yield stress estimated by the RC Taylor
 427 model. This equation allows us to immediately correct the value of τ_{ini} without any
 428 identification procedure. Once the beginning of the curve has been correctly adjusted, we can
 429 repeat the procedure for the saturation stress, by considering that, if this level is not reached
 430 on the experimental curves, it can be again correctly identified by the RC Taylor model,
 431 which means $(\sigma_{sat})_{Tay} \cong (\sigma_{sat})_{exp}$. The result of a 2nd Abaqus simulation (*sim2*) performed

432 with h_{01} , τ_{ini} , τ_{sat1} allows us to write

$$\frac{(\sigma_{sat})_{Tay}}{\tau_{sat}} = \frac{(\sigma_{sat})_{sim2}}{\tau_{sat1}} \quad (20)$$

433 and to obtain the correct value of τ_{sat} again without any identification procedure. It is worth
434 noting, that this step implies to be able to perform one simulation with RC Taylor and one
435 simulation with Abaqus up to the saturation level. This may involves convergence problems
436 with Abaqus (especially if the saturation level is reached at very high strains). In this case, a
437 classical identification procedure will have to be applied. In any case, there remains then one
438 single parameter to be identified, which is again the hardening coefficient h_0 . The procedure
439 is summarized in Table III and illustrated in Figure 9. It is seen that the agreement between
440 experimental and predicted curves is again quite satisfactory. Again, like for the RC Taylor
441 model, some other materials parameters can be recalculated if we change the value of γ_0
442 without being obliged to perform the simultaneous identification of all parameters.

443

444 ***4.3 Case study 3: the transition between static and dynamic regimes***

445 The previous cases have illustrated clearly the fact that the macroscopic response of a
446 polycrystalline aggregate strongly depends on both normalized strain rate (ratio of imposed
447 over reference strain rates) and strain-rate sensitivity exponent; especially, the only
448 configuration where a strain rate independent limit can be reached is for $\dot{E}_{VM} = \gamma_0$, with n
449 greater than 20). This is true when using simple mean field models such as the RC Taylor one
450 (used here) as well as more complex full field tools such as FE codes. However, when FE
451 simulations are performed, the strain rate, and thus the strain-rate sensitivity, can significantly
452 vary from one point to another, as recently underlined by Shahba and Gosh [10] who studied
453 the behavior of strongly anisotropic Ti alloys; in that case, the choice of the viscoplastic
454 parameters γ_0 and n is not so trivial **if we want**, e.g., to neglect the influence of strain rate in
455 the whole sample. If one single macroscopic strain rate is investigated (and if the fluctuations
456 within the simulated structure are expected to be moderate enough), then taking $\dot{E}_{VM} = \gamma_0$
457 allows to neglect the strain rate sensitivity as much as possible and to select a n exponent as
458 small as possible to reduce the computation time, without going to extensive multiple slip due
459 to overestimated viscosity. Typically, a value around 20 satisfies these constraints and the
460 hardening parameters can then be simply identified on one experimental curve (as done in the
461 present case for the 304L material). But if several values of macroscopic or microscopic strain
462 rate need to be considered, then the selection of the two parameters can be made according to

463 several procedures:

464 (i) As suggested by Khan et al. [9], it is possible to arbitrarily select for $\dot{\gamma}_0$ one of the
465 investigated values of strain rate and to identify the hardening parameters on the
466 corresponding curve and then, to identify the n exponent on the curves obtained for the
467 other strain rates. According to these authors however, this option is not completely
468 satisfactory if the associated hardening law is too simplified, as the one used in the
469 present work, since they argue that it is not possible in this case to reproduce all
470 experimental curves obtained e.g. on **aluminum** single crystals over a wide range of strain
471 rate with one single n parameter. They then propose to select a more complex hardening
472 law, which comprises an additional strain rate sensitivity parameter. It is worth
473 mentioning though that the behavior of the tested Al single crystals observed at varying
474 strain rates is somewhat in contradiction with the conclusions drawn recently by Shahba
475 and Gosh [10] who claimed that in general (and not only for the Ti alloys), the classical
476 phenomenological power law is valid up to larger strain rates (up to 10^4 s^{-1}) than the ones
477 investigated by Khan et al. [8], which do not exceed 10^3 s^{-1} .

478 (ii) Alternatively, it can be recognized, as suggested by Canova et al. already in 1988 [1] and
479 more recently by Uenishi and Teodosiu [55] or by Shahba and Gosh [10], that one single
480 n parameter cannot reproduce all observed behaviors and that there are indeed three
481 different regimes:

- 482 1. the quasi-static regime associated with strain rates below 1 s^{-1} ,
- 483 2. the dynamic regime associated with strain-rates typically above 100 or even 1000 s^{-1}
484 – depending on the authors – these two regimes being associated either with
485 significantly different values of n or with different VP flow rules and even different
486 hardening mechanisms [10, 55],
- 487 3. the transition regime between the two, within which the n value may vary more or
488 less smoothly.

489 To describe this evolution from quasi-static to dynamic regime, Canova et al. [1] proposed a
490 bilinear expression for the evolution of the true stress as a function of the strain rate whereas
491 Uenishi and Teodosiu [55] proposed a parabolic expression, taking into account the effect of
492 temperature within the dynamic regime. As for Shahba and Gosh [10], they propose a so-
493 called unified flow-rule, applicable to a very wide range of applied strain-rates and
494 temperatures, “uniquely capable of seamlessly accounting for the effects of location-
495 dependent thermally-activated (at low strain rates) and drag-dominated (at high strain rates)

496 mechanisms of dislocation glide without any user intervention”. Their law is thus especially
497 well adapted to FE simulations performed for very high strain rates, for which strain rates at
498 different locations in a heterogeneous polycrystalline microstructure are expected to vary
499 significantly even for a uniformly applied macroscopic strain-rate.

500 If the existence of two different regimes (and possibly of a smooth transition between the
501 two) is thus well recognized, it is then easy to conclude that the use of the classical VP flow
502 rule with one single set of parameters (describing both flow and hardening rules) should be
503 allowed within one of these two regimes only. As long as the influence of temperature is not
504 explicitly included, as e.g. in the phenomenological hardening law selected in the present
505 work, it is also easy to recognize that the present formulation is thus more adapted to the
506 quasi-static regime than to the dynamic one (for which additional microscopic deformation
507 mechanisms are expected to occur). In this case, the value of $\dot{\gamma}_0$ should also be selected within
508 the quasi-static regime, which means typically below 1 s^{-1} . If the parameters are identified as
509 previously explained, it is then possible to reproduce the behavior of a material within the
510 whole quasi-static regime with one single set of parameters, as already illustrated for
511 polycrystalline aluminum in section 4.2 but also for Al single crystals, as illustrated in Figure
512 10: the experimental curves obtained on Al single crystals deformed in compression by Khan
513 et al. [9] have been reproduced with the RC Taylor model (see parameters in Table IV). It is
514 seen that the 3 curves corresponding to the quasi-static regime are well reproduced (even
515 better than in the original paper with a different, although also phenomenological hardening
516 law) whereas the one associated with the dynamic regime (strain rate equal to 1000 s^{-1}) is not
517 with the quasi-static parameters. If now the n exponent is allowed to be modified for the
518 dynamic regime, then the curve can also be reproduced with the simple RC Taylor model and
519 saturating hardening law. It is worth mentioning though, that the strain-rate sensitivity ($1/n$)
520 is observed here to decrease at high strain rate, in contradiction with most of the other
521 observations performed in metals [1, 10, 20, 33, 55, 56]. The reason for this quite unusual
522 dynamic behavior of the tested Al single crystals is not explained in ref. [8].

523

524 **6. Conclusions**

525

526 The aim of the present study was to rationalize the use of the simple VP power law, still
527 widely used for its simplicity with mean field and full field approaches to model the behavior
528 of polycrystalline samples in a wide range of strain-rates or temperatures. For this purpose,

529 one mean field (RC Taylor model) and one full field (Abaqus FE code) approaches have been
530 selected, with the very same description of the single crystal behavior (fcc in the present
531 case). These two approaches have been selected since they can predict heterogeneities of
532 strain, stress and strain rate within a polycrystalline sample, as experimentally observed. As a
533 consequence, the conclusions drawn below are thought to be also applicable to other
534 modelling choices. Through the simulation of simple tensile tests and the comparison of some
535 simulated and experimental curves, we have shown that:

- 536 (i) with such a rate-sensitive single crystal constitutive law, **it is possible to simulate**
537 **the behavior of rate-sensitive or rate-insensitive materials, in the framework of**
538 **both mean field or full field approaches, provided that it is remembered that** the
539 macroscopic response of a polycrystalline aggregate will depend on both values
540 selected for the reference strain rate $\dot{\gamma}_0$ with respect to the imposed one and the
541 strain-rate sensitivity exponent n ;
- 542 (ii) **for rate-insensitive materials**, the strain-rate exponent value which allows to
543 approximate the rate-insensitive limit with sufficient precision depends on the
544 macroscopic strain rate, as long as the $\dot{\gamma}_0$ parameter has been selected. If $n = 21$
545 is high enough for a strain rate equal to $\dot{\gamma}_0$, much higher values must be selected,
546 as soon as the strain rate is modified; as a consequence, even for $n = 21$ and
547 $\dot{E}_{VM} = \dot{\gamma}_0$, some strain rate sensitivity can be observed within individual grains, as
548 long as the deformation is not prescribed to be uniform within the whole
549 polycrystalline sample and that strain-rate variations are thus observed; today, this
550 is well-known only by a limited part of the FE code users;
- 551 (iii) the VP formulation with one single exponent and associated with a simple
552 hardening law neglecting the temperature effects, is quite adequate to describe the
553 quasi-static regime, i.e. typically for strain rates below 1/s (or below $\dot{\gamma}_0$), for rate-
554 sensitive materials; once all parameters have been identified for one reference
555 case, it is then easy to modify them to treat another reference case. It has been
556 shown that the identification procedure can be considerably simplified in this case,
557 since 2 of the 3 hardening parameters can simply be corrected without any
558 identification procedure;
- 559 (iv) **the identification of all parameters of the constitutive law with an FE code can be**
560 **greatly accelerated by relying on the identification previously carried out with a**
561 **simpler model, such as the RC Taylor model.**

562 (v) The simple VP formulation studied here can also be used to describe the behavior
563 of rate-sensitive material in an extended range of strain-rate (i.e. including both
564 static and dynamic regimes), provided that the exponent n is identified separately
565 in both regimes.

566 Finally, it is worth recalling that this widely used VP formulation is phenomenological. It
567 is thus not adequate to describe completely all the microscopic mechanisms. If this is
568 desired, this simple formulation should be enriched to account for a more precise
569 description and more detailed understanding of strain rate and temperature effects.

570

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584

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586

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Table I. Imposed and adjusted parameters for the identification of the 304L experimental curve with the RC Taylor model.

Imposed test conditions (reference case)	$\dot{E}_{VM} = \dot{E}_{33imp} = 0.001 s^{-1}$ $E_{33max} = 0.35$
Imposed parameters	$\dot{\gamma}_0^s = \dot{\gamma}_0 = 0.001 s^{-1}$ $n = 21$
Material adjusted parameters	$\tau_0^s = 100 MPa$ $h_0 = 260 MPa, q = 1.1$ $\tau_{sat} = 300 MPa, \tau_{ini} = 100 MPa$

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Table II. Imposed and adjusted parameters for the identification of the aluminum experimental curves with the RC Taylor model.

$\dot{E}_{VM} (s^{-1})$ for the identified curve	Imposed parameters			Adjusted parameters		
	n	$\dot{\gamma}_0 (s^{-1})$	q	h_0 (MPa)	τ_{ini} (MPa)	τ_{sat} (MPa)
0.0005	15	0.0005	1.1	4	15	35
0.05	15	0.05	1.1	5.7	20	47

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Table III. Imposed and adjusted parameters for the identification of the aluminum experimental curves with the Abaqus FE code.

Simulation	Fixed parameters $n = 15, \dot{E}_{VM} = \dot{\gamma}_0 = 0.0005 s^{-1}, q = 1.1$			
	Parameters to be identified	h_0 (MPa)	τ_{ini} (MPa)	τ_{sat} (MPa)
<i>sim1</i> (up to σ_0)	$h_{01}, \tau_{ini1}, \tau_{sat1}$ issued from the RC Taylor identification	4	15	35
<i>sim2</i> (up to σ_{sat})	τ_{ini} corrected by Eq. 19 h_{01}, τ_{sat1} issued from the RC Taylor identification	4	14	35
<i>sim3</i> (up to $\sigma_{expfinal}$)	τ_{sat} corrected by Eq. 20 Identification of h_0 with Abaqus	5	14	45

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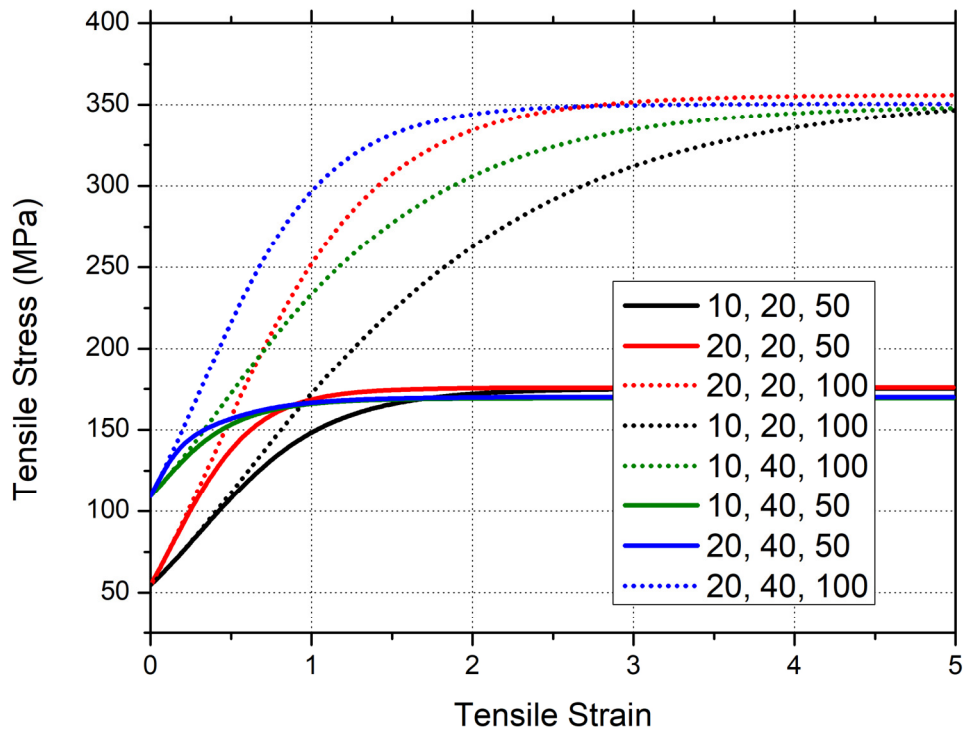
755 Table IV. Imposed and adjusted parameters for the identification of the Al single crystals
 756 compression curves of Khan et al. [9] with the RC Taylor model.
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Imposed test conditions	$\dot{\epsilon}_{VM} = \dot{\epsilon}_{33imp} = 1 \text{ to } 0.001 \text{ s}^{-1}$ (quasi-static) $\dot{\epsilon}_{VM} = \dot{\epsilon}_{33imp} = 1000 \text{ s}^{-1}$ (dynamic)
Reference case for identification of the material parameters	$\dot{\epsilon}_{33imp} = 1$
Imposed parameters	$\dot{\gamma}_0^s = \dot{\gamma}_0 = 1 \text{ s}^{-1}$ $n = 21$ (quasi-static), $n = 41$ (dynamic)
Adjusted parameters	$\tau_0^s = 5 \text{ MPa}$ $h_0 = 40 \text{ MPa}, q = 1.1$ $\tau_{sat} = 35 \text{ MPa}, \tau_{ini} = 5 \text{ MPa}$

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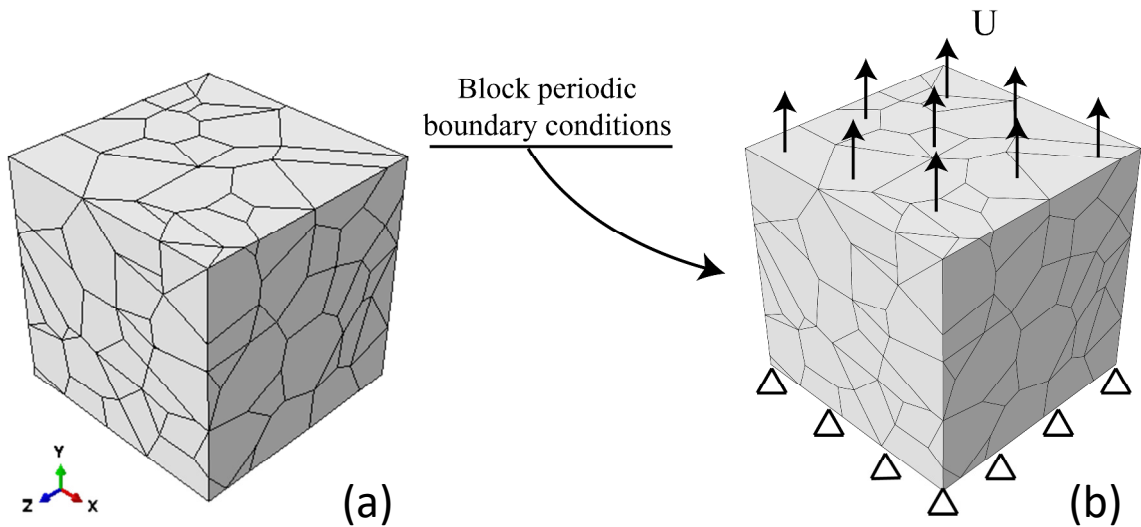
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Figure 1. Simulated tensile curves using the RC Taylor model, with $\dot{\gamma}_0^s = \dot{\gamma}_0 = \dot{\epsilon}_{VM} = 0.0005 \text{ s}^{-1}$, $q = 1.1$ and $n = 21$. The 3 hardening parameters h_0 , τ_{ini} , τ_{sat} are varied and their values (in MPa) given in the figure legend.

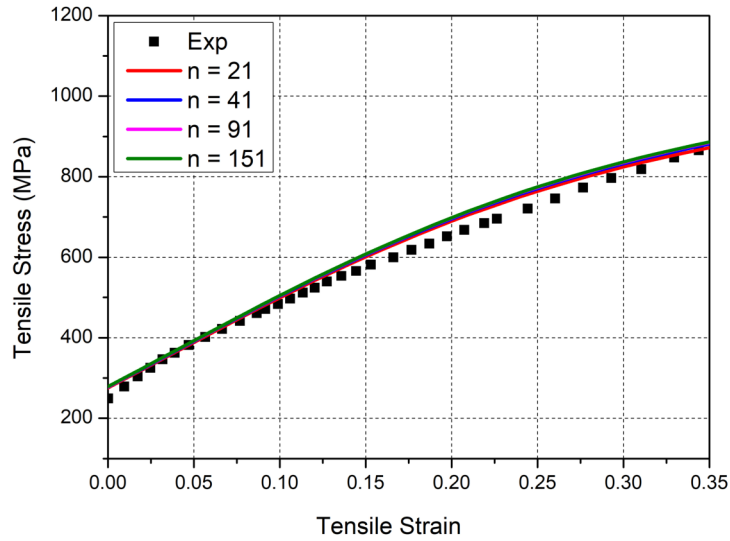


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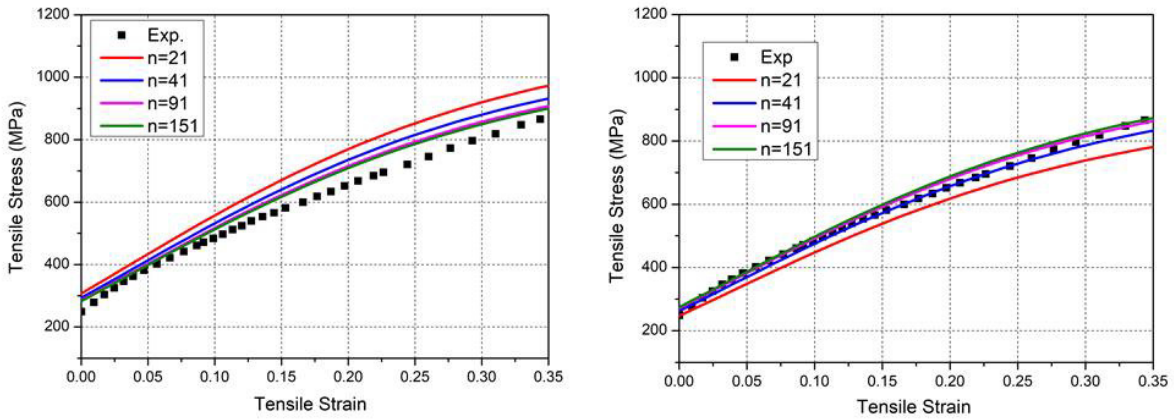
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Figure 2. (a) Example of a Voronoi tessellation made of 200 grains and (b) applied boundary conditions.



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Figure 3. Tensile curves obtained with the RC Taylor model for the reference case ($\dot{E}_{33imp}/\dot{\gamma}_0 = \dot{E}_{VM}/\dot{\gamma}_0 = 1$) and various n values. Comparison with the experimental curve obtained by Chavez et al. [46] on a 304L stainless steel at room temperature.

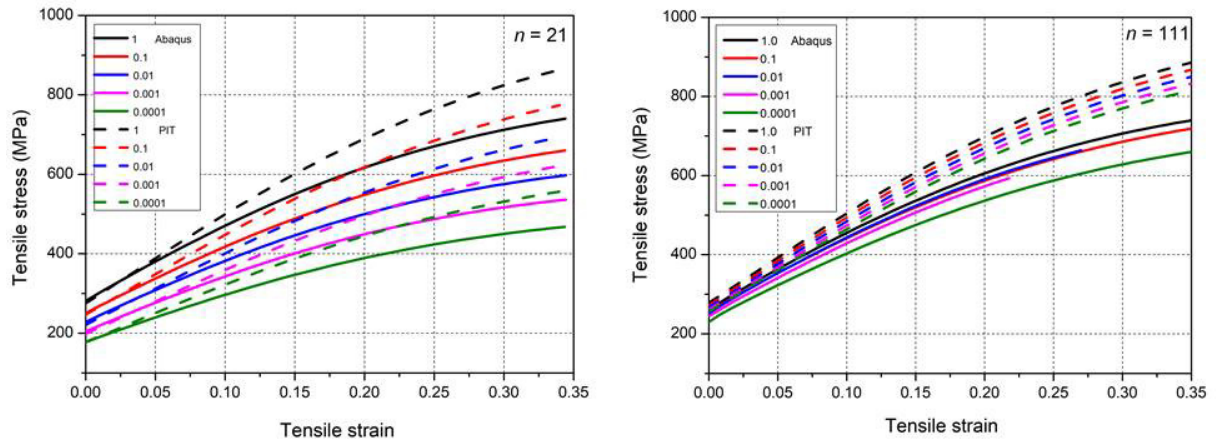


(a) $\dot{E}_{VM}/\dot{\gamma}_0 = 1/10$

(b) $\dot{E}_{VM}/\dot{\gamma}_0 = 10$

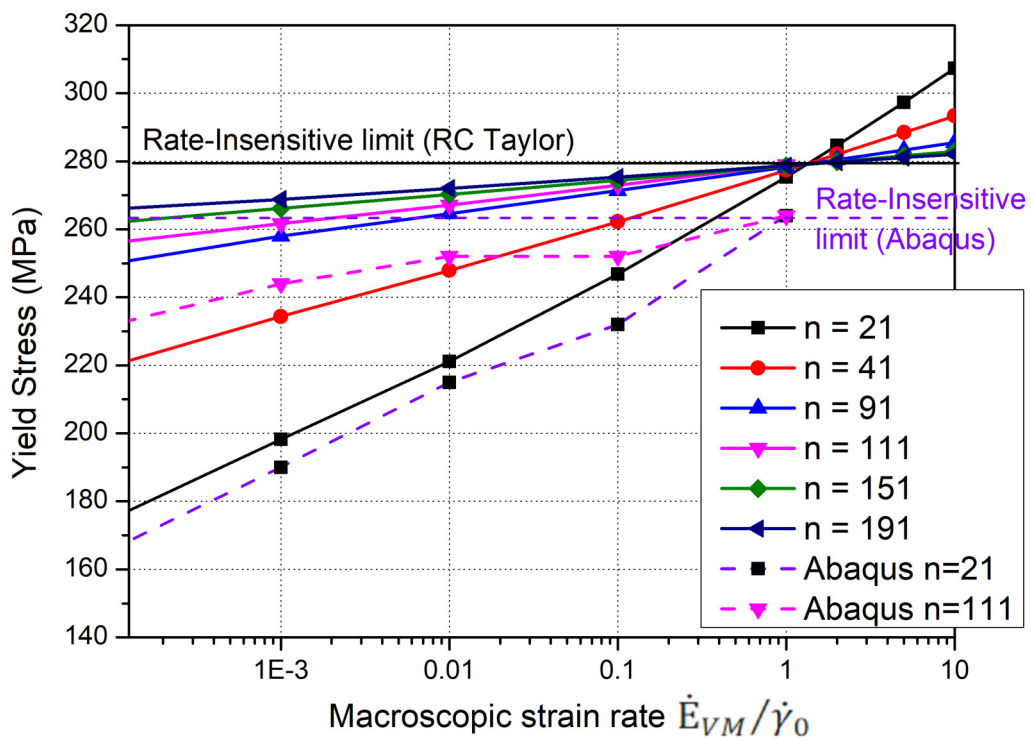
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Figure 4. Tensile curves obtained with the RC Taylor model for 2 test parameter sets different from the reference case, and various n values. Comparison with the experimental curve obtained by Chavez et al. [46] on a 304L stainless steel at room temperature.



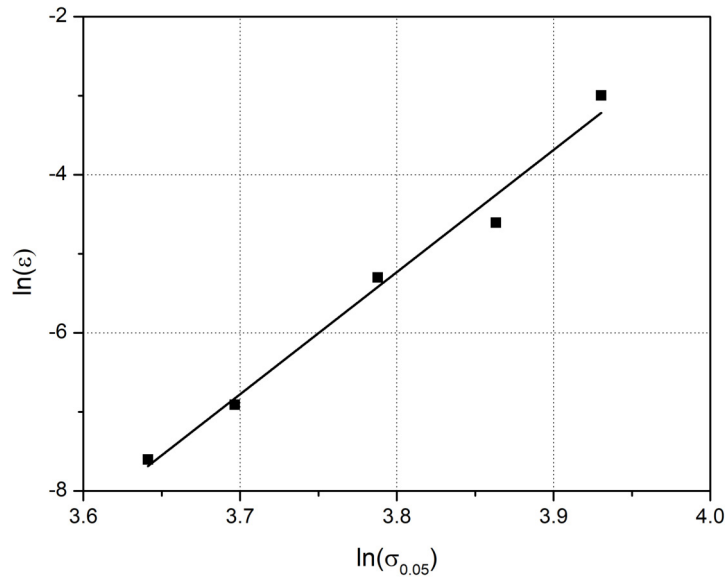
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Figure 5. Tensile curves obtained with the RC Taylor model and the Abaqus code for 5 different applied normalized strain rate values (from 0.0001 up to 1 s^{-1}) and $n=21$ or 111.



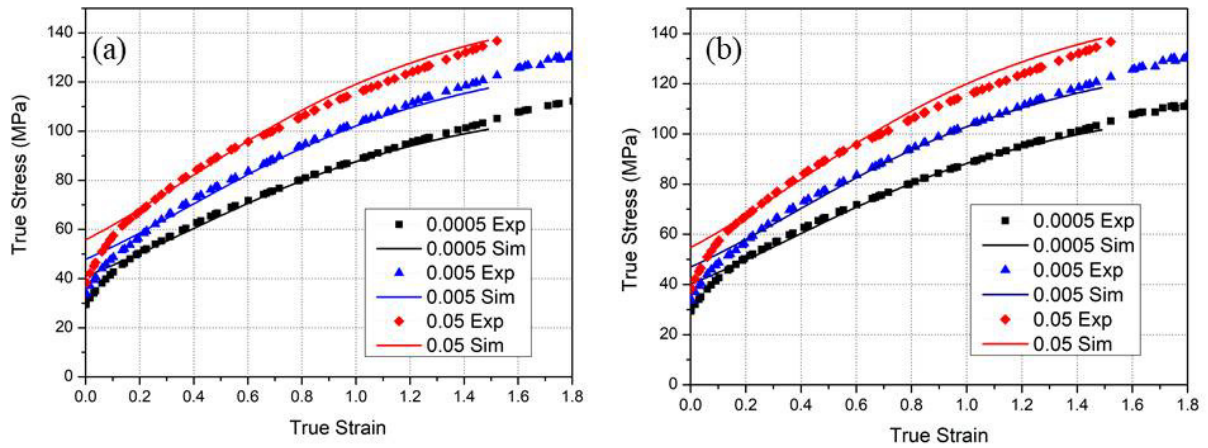
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Figure 6. Evolution of the macroscopic yield stress as a function of strain rate and strain-rate sensitivity exponent for all performed simulations.



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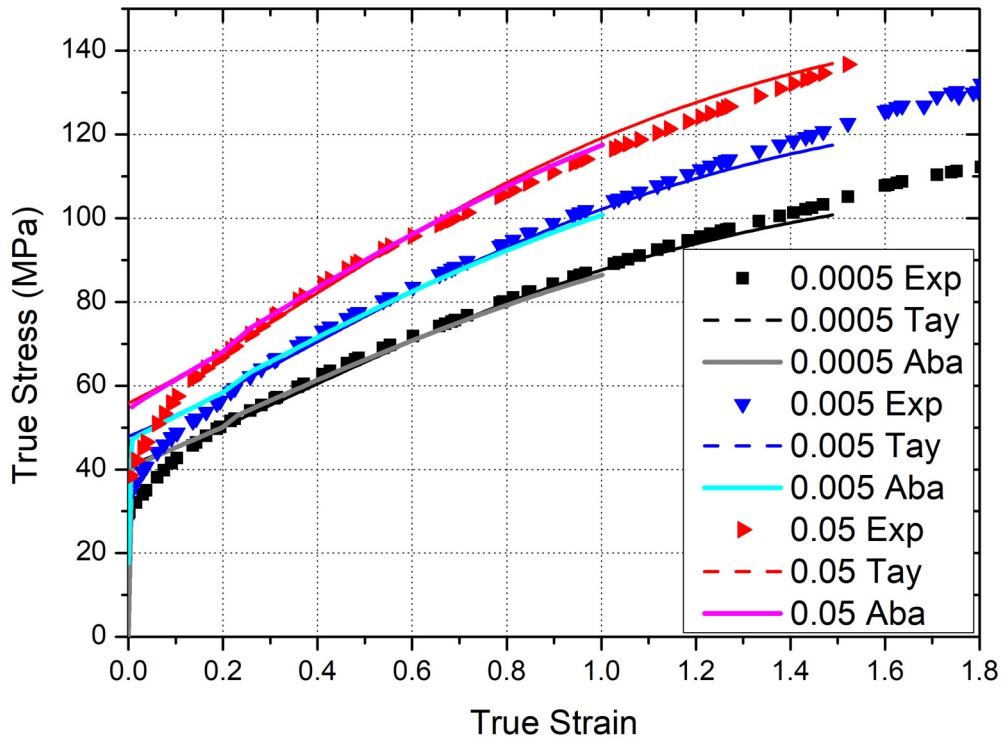
Figure 7. Relationship between strain rate and yield stress extracted from experimental tensile curves obtained on pure aluminum at room temperature [54].



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Figure 8. Stress – strain curves obtained for pure aluminum deformed in tension at various strain rates. The experimental curves are taken from [54] and the simulated ones are obtained with the RC Taylor model, using 2 sets of parameters (see Table II):

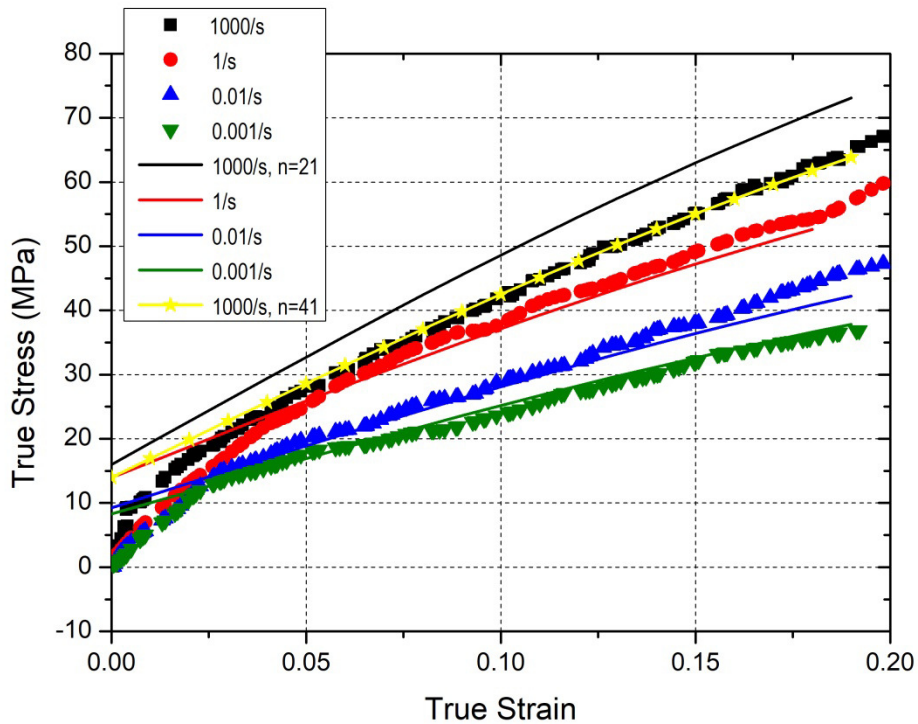
(a) $\dot{\gamma}_0 = 0.0005 \text{ s}^{-1}$ and (b) $\dot{\gamma}_0 = 0.05 \text{ s}^{-1}$.



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813 Figure 9. Stress – strain curves obtained for pure aluminum deformed in tension at various
 814 strain rates. The experimental curves are taken from [53] and the simulated ones are obtained
 815 with the RC Taylor model (parameters in Table II) and with the Abaqus FE code, with the
 816 hardening parameters listed in Table III, evaluated with the proposed identification method.

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819 Figure 10. Experimental (dotted lines from [9]) and simulated (full lines, RC Taylor model)
 820 curves for Al single crystals deformed in compression.