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2 **A new macroscopic strain hardening function based on microscale crystal plasticity**

3 **and its application in polycrystal modeling**

4

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14

15 **Abstract**

16 A new phenomenological strain hardening function is proposed to describe the strain
17 hardening behavior of metallic materials. The function is based on a simplification of an
18 earlier established self and latent hardening crystal plasticity approach. The proposed
19 function contains only four parameters, which can be readily obtained using an efficient
20 numerical technique by fitting the experimental curve. Several applications on different
21 materials are presented and good agreements with the experimental counterparts were
22 obtained. One great advantage of the proposed empirical function is that its parameters can be
23 directly used in polycrystal viscoplastic modeling (VPSC approach) for crystal plasticity-
24 based incremental strain hardening simulations. For the conversion of the parameters between
25 the macroscopic scale and the grain-level, the Taylor factor was used, which was re-defined
26 for polycrystals in the present work. The VPSC simulations also led to good reproduction of
27 the experimental strain hardening behavior for all investigated cases, with rapid convergence.

28 **Keywords:** Strain hardening, Phenomenological function, Polycrystal plasticity, VPSC
29 modeling

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31 1. Introduction

32 Strain hardening is considered to be one of the most important strengthening
33 mechanisms as it plays a critical role in evaluating the material's functional properties and
34 determines its suitability for engineering/structural applications. In general, such a
35 characteristic response is obtained experimentally from the macroscopic response of a
36 specimen loaded under simple compression, tension, or shear in the form of a stress-strain
37 curve. Depending on material properties (such as crystal structure, grain size, etc.) and
38 imposed loading conditions, the shape of a stress-strain curve varies significantly and
39 frequently shows distinct stages [1-8]. In this aspect, finding a suitable empirical function that
40 can reproduce the experimental measurements is a challenging task and has been the subject
41 of numerous investigations. Indeed, analytical functions are useful in assessing material
42 performance for design purposes.

43 Under this premise, well-known and widely used classical constitutive relations either
44 follow a power-law or an exponential form. Examples for the former were suggested by
45 Ludwik [9], Hollomon [10], and Swift [11], while the Voce-approach [12] was proposed for
46 the latter. The drawback of the mentioned power-law form approaches is that there is no
47 upper limit for the flow stress, while a final saturation stage of strain hardening is frequently
48 observed, especially during severe plastic deformation [3]. To account for the saturation
49 stress, the exponential form of the Voce-equation [12] has received special attention in which
50 the flow stress approaches an asymptotic value at a high strain level. Subsequently, several
51 approaches were proposed in this context that used an increased number of fitting parameters
52 to capture the stress-strain response [1,13]. Chinh et al. [3] introduced an exponential power-
53 law constitutive relationship that reduces to the conventional Hollomon power-law
54 relationship at low strains and to the Voce exponential relationship at high strains. They
55 demonstrated that the approach was effective in capturing the stress-strain relationship of
56 high purity aluminum and copper over a wide range of strain, however, non-negligible
57 deviations still existed in their findings for high strains. Recently, Lavakumar et al. [7]
58 presented an improved empirical version of the Ludwigson [1] equation with additional terms
59 and fitted parameters and applied successfully to several materials. Other approaches were
60 based on the physical deformation mechanisms observed at the dislocation scale, for
61 example, the Kocks-Mecking approach, which is very suitable for Stage III hardening [14-16]
62 and the dislocation cell-based theory of Estrin et al. [2] to reproduce Stages III and IV.

63 Besides, the fit of an experimental stress-strain curve is also possible by crystal
64 plasticity-based approaches where the parameters refer to strain hardening of individual slip
65 systems, capable of distinguishing self and latent hardening [17-20] using a power-law
66 relation with a saturation stress. Such physically-based approaches have proven to be
67 effective for many materials and are well suited for a wide variety of loading conditions as
68 well as deformation to large strain regimes (for example: Zhou et al. [19]; Wu et al. [21];
69 Dhinwal and Toth [22]; Sahoo et al [23]; Vu et al. [24]). Nevertheless, one of the challenges
70 of such approaches is to determine the optimal values of the crystal plasticity-based strain
71 hardening parameters. In this regard, various experimental [25-27] and computational [28-31]
72 optimization methodologies were suggested to identify an optimal set of material hardening
73 parameters for crystal plasticity models. The most conventional approach for identifying
74 crystal plasticity hardening parameters is to carry out simple mechanical tests on a single
75 crystal [25,26]. However, this is seldom practiced as most of the materials are often available
76 as polycrystals, and the boundary conditions are very different for a crystal embedded into
77 the polycrystal. A usual way is to use the inverse analysis technique which involves
78 calibrating the material parameters until the simulation results match the experimental data.
79 This is primarily based on the least-square method or simply using a trial-and-error approach.
80 The former refers to an optimization process where a set of parameters is recognized for an
81 objective function that minimizes the variance between the experimental data and the
82 computed response. While the latter corresponds to a manual searching of each parameter by
83 iteratively fitting the experimental curve. However, both of these approaches require initial
84 estimation of the parameter values and involve a large number of iterations in an effort to
85 converge to an optimal solution. At the same time, such techniques reflect two key sources of
86 ambiguity for the quantitative estimation of parameters: (i) *uncertainty*, which occurs because
87 of the presence of numerous associated unknown parameters within the phenomenological
88 constitutive law, such that the effect of one parameter can be compensated by the other set of
89 parameters on the course of strain hardening, and (ii) *inconsistency*, because the obtained
90 values of the parameters are arbitrary. Consequently, to validate the experimental findings,
91 these techniques are very complex and usually it is difficult to interpret the physical meaning
92 of the parameters.

93 Therefore, to exploit the full predictive potential of the adjustable hardening
94 parameters in a single expression, it is necessary to establish a meaningful and optimized set
95 of hardening parameter values. With the advancement in computational technology, several

96 researchers have proposed inverse analysis strategies for the computational optimization
97 algorithm by employing sophisticated experimental techniques [32-39]. The experimental
98 results can be achieved by the most commonly available instrumented techniques such as
99 nano-indentation or digital image correlation (DIC). The former involves probing individual
100 grains within the polycrystal and extracting the indentation stress-strain response in the form
101 of the load-displacement curve for several grains within the polycrystal, which is then used to
102 construct the macroscopic response [32-37]. In this regard, Patel et al. [35] utilized spherical
103 indentation to establish a correlation between the indentation stress-strain curve and the
104 uniaxial stress-strain curve via simple scaling factors. Subsequently, they validated these
105 scaling factors using a finite element (FE) model. Mandal et al. [36] established a canonical
106 correlation analysis to explain the influence of the constitutive model parameters on the flow
107 stress behavior within the framework of the mechanical threshold stress (MTS) model [40].
108 However, owing to the complex stress state beneath the indenter, it is difficult to interpret the
109 experimental results and obtain the parameters that govern the hardening behavior. Also,
110 these experimental strategies are very time-consuming as the number of experiments to be
111 carried out on several grains is large, and incurs a huge experimental cost, with an additional
112 drawback of the indentation size-effect.

113 Alternatively, within the framework of experimental techniques, DIC enables the
114 measurement of spatial displacement and strain fields and provides an insight into the
115 micromechanics of solids. Guery et al. [38] used the inverse analysis technique for coupling
116 the experimentally measured spatial strain fields produced via DIC and the weighted finite
117 element modeling update (FEMU) scheme for qualitative estimation of the crystal plasticity
118 parameters. The FEMU approach is based on comparing the results of FE modeling with
119 experimental results, by minimizing the error. However, to converge into an acceptable
120 solution, the method requires numerous FEM calculations. Despite these advancements, a
121 time-efficient methodology is always sought which could overcome the computational cost
122 and at the same time provide an approximation to the values of the uncertain parameters
123 present in the strain hardening functions.

124 Based on this perspective, the present investigation is undertaken with two major
125 objectives: (i) A new analytical version of the strain hardening function based on a power-law
126 relation is proposed, which has its origins in crystal plasticity. Unlike all other existing
127 empirical power-law functions, this power-law function is unique in the sense that it has
128 saturation stress that can drive the flow stress to saturation. (ii) A suitable minimization

129 technique is proposed for determining the optimal values of the unknown hardening
130 constants. The reliability of the proposed approach was tested critically by applying it to
131 different materials: Aluminum, Copper, Steel, and Titanium, undergoing various deformation
132 modes, such as tensile, compression, as well as torsion testing, and demonstrated good fitted
133 response. To this end, the parametric values obtained from the proposed procedure were also
134 employed in a crystal plasticity framework, which includes much more physics on the
135 deformation of the polycrystal than a phenomenological function. The VPSC (viscoplastic
136 self-consistent) polycrystal model was used for this purpose, and the obtained strain
137 hardening was also in good agreement with the experiments, like the phenomenological one.
138 The great advantage of doing first a phenomenological fitting before the VPSC simulation is
139 that the phenomenological parameters serve as an excellent initial guess for the crystal
140 plasticity simulations. In this way, the VPSC simulation work is highly reduced, and the
141 obtained results are remarkable.

142

143 2. The principles of the new strain hardening function

144 In crystal plasticity, strain hardening is frequently modeled using self and latent
145 hardening of the slip systems. One of the frequently used approach was introduced by
146 Kalidindi et al. [18], then later modified by Zhou et al. [19]. It expresses the influence of all
147 slip systems on the hardening rate of a given slip system ‘*i*’ and is given by:

$$148 \quad \dot{\tau}_0^i = \sum_{j=1}^n q_c^{ij} h_c \left(1 - \frac{\tau_0^j}{\tau_{sat}^j} \right)^{a_c} |\dot{\gamma}^j|. \quad (1)$$

149 Here, τ_0^i is the resolved shear stress in slip system *i*, $\dot{\gamma}^j$ is the resolved shear strain rate in the
150 slip system *j*, and *n* is the total number of slip systems. q_c^{ij} denotes a (*n* x *n*) matrix and
151 accounts for the self and latent interactions between the slip systems (the index ‘*c*’ stands for
152 ‘crystal plasticity’). The diagonal elements of q_c^{ij} represent the effect of self-hardening, while
153 the off-diagonal parts are the latent hardening terms [17]. h_c and a_c are the hardening
154 parameters, and τ_{sat}^i denotes the saturation stress. The essential novelty of the present work
155 is to use an analytical version of this hardening rule, applicable at the macroscopic level:

156
$$\dot{\sigma}_0(\bar{\epsilon}) = h \left(1 - \frac{\sigma_0(\bar{\epsilon})}{\sigma_{sat}} \right)^a \bar{\dot{\epsilon}}. \quad (2)$$

157 Here $\bar{\dot{\epsilon}}$ is the macroscopic von-Mises equivalent strain rate and σ_0 is the reference strength
 158 of the material, which appears in the strain rate sensitive power-law formula of viscoplastic
 159 behavior:

160
$$\sigma(\bar{\epsilon}) = \sigma_0(\bar{\epsilon}) \left(\frac{\bar{\dot{\epsilon}}}{\dot{\epsilon}_0} \right)^m, \quad (3)$$

161 with m being the macroscopic strain rate sensitivity index and $\dot{\epsilon}_0$ the reference strain rate.

162 It should be noted here that in the above formulation, the self and latent hardening have been
 163 simplified and thus, do not appear in the formula. Also, while there can be several different
 164 values for τ_{sat}^i in Eq. (1), the macroscopic curve can contain only one parameter for the
 165 saturation stress; σ_{sat} . After separating the variables and integrating Eq. (2), the following
 166 form of the strain hardening function can be obtained:

167
$$\sigma_0(\bar{\epsilon}) = \sigma_{sat} - \sigma_{sat} \left[\left(\frac{h(a-1)}{\sigma_{sat}} \right) \bar{\epsilon} + \left(1 - \frac{\sigma_{00}}{\sigma_{sat}} \right)^{1-a} \right]^{\frac{1}{1-a}}, \text{ where } a \neq 1. \quad (4)$$

168 Here σ_{00} is the yield strength of the material (at $\bar{\epsilon} = 0$). The number of unknown
 169 parameters in this function is four; they are: σ_{00} , σ_{sat} , h , and a . Among these, σ_{00} can be
 170 readily assigned from the experiment. While the values of the remaining three parameters
 171 (i.e., σ_{sat} , h , and a) cannot be assigned directly; they need to be identified from the
 172 experimental curve using a suitable fitting procedure. A relatively simple and fast procedure
 173 is a minimization technique, which is presented in the next section.

174

175 3. Parameter identification procedure

176 The first parameter is the yield stress (σ_{00}), thus the flow stress value at the
 177 beginning of the plastic strain ($\epsilon = 0$). To obtain the other three parameters, a large number of

178 co-ordinate points were selected on the experimental flow stress curve; typically, about $N=50$,
 179 and the following scalar function was defined:

$$180 \quad f = \sum_{i=1}^N \left| \sigma_i^{sim}(\bar{\epsilon}_i) - \sigma_i^{exp}(\bar{\epsilon}_i) \right| = \min. \quad (5)$$

181 Here the superscripts ‘*sim*’ and ‘*exp*’ stand for the stress value from Eq. (4), and the
 182 experimental one, respectively. An efficient procedure for minimizing this function is to
 183 employ a suitable bracketing technique until the function’s value (f) approaches zero with the
 184 specified precision. To begin the bracketing process, large initial intervals were defined for
 185 each of the three parameters. In the current study, the intervals of the parameters were: $\sigma_{sat} \in$
 186 $[\sigma_{00}, 1000 \text{ MPa}]$, $h \in [0, 100000 \text{ MPa}]$, and $a \in [1, 10, a \neq 1]$. At the very beginning, each of
 187 these intervals were divided into 100 equal intervals and the function values f were calculated
 188 for all possible combinations of the 100^3 parameter values, then the parameter combination
 189 corresponding to the minimum f value was identified. Subsequently, in the next iteration, the
 190 same procedure was repeated on the reduced intervals (which were divided into 100
 191 intervals), and the cycle continued several times, until the minimum f value reached the
 192 required precision (0.01 MPa). The mentioned procedure is computationally very fast, it
 193 converges in seconds to achieve the specified precision [see the Fortran program as an
 194 additional available material at *LaszloSToth/Hard-fit-by-minimization: An efficient Fortran*
 195 *program to fit a stress-strain curve by the empirical function derived from crystal plasticity.*
 196 (*github.com*)].

197 For the special case, when $a = 1$, we obtain from Eq. (2):

$$198 \quad \sigma_0(\bar{\epsilon}) = \sigma_{00} + h' \cdot \bar{\epsilon}, \quad \text{where } h' = h \cdot \left(1 - \frac{\sigma_{00}}{\sigma_{sat}} \right). \quad (6)$$

199 So, for $a = 1$, the strain hardening is linear. Therefore, for linear hardening, the meaning of
 200 the σ_{sat} parameter is not a saturation stress, it is just a parameter with stress dimension. In
 201 this case, only one point is needed from the experimental curve to obtain the value of the h'
 202 parameter (if σ_{00} can be read from the experimental curve).

203 The proposed new function in Eq. (2) can only describe hardening, because the term
 204 $\left(1 - \frac{\sigma_0(\bar{\mathcal{E}})}{\sigma_{sat}}\right)$ must be positive. Softening corresponds to $\sigma_{sat} \leq \sigma_0(\bar{\mathcal{E}})$. In this case, the
 205 integration of Eq. (2) leads to the following:

$$206 \quad \sigma_0(\bar{\mathcal{E}}) = \sigma_{sat} + \sigma_{sat} \left[\left(\frac{h(a-1)}{\sigma_{sat}} \right) \bar{\mathcal{E}} + \left(\frac{\sigma_{00}}{\sigma_{sat}} - 1 \right)^{1-a} \right]^{\frac{1}{1-a}}, \quad (\text{for softening: } \sigma_{sat} \leq \sigma_{00}). \quad (7)$$

207

208 **4. Use of the macroscopic hardening parameters in polycrystal plasticity** 209 **simulations**

210 One of the main goals of the proposed methodology is to evaluate and assess the
 211 identified hardening parameters so that they can be conveniently used in crystal plasticity
 212 simulations. Indeed, it is a challenging task to perform a high-quality numerical work for
 213 simulating the macroscopic strain-hardening behavior of polycrystals with crystal plasticity
 214 approach. Nevertheless, it is often successful, as there are excellent simulation results
 215 published in several studies [22-24, 41-45]. The usual technique used is trial and error, which
 216 requires many iterations. However, when there are initial parameters that are already good
 217 approximations, the task becomes much more efficient. Indeed, as the proposed macroscopic
 218 strain hardening function was obtained by simplifying a microscopic (crystal plasticity)
 219 modeling function, it is possible to use the macroscopic parameters as a good initial guess for
 220 the crystal plasticity simulations.

221 There are differences between the values of the macroscopic and microscopic
 222 hardening parameters which are due to the difference in the scale of the mechanical behavior.
 223 Therefore, one has to link the two scales. One possibility is to use the Taylor factor which
 224 relates stress and strain between the two scales. The Taylor factor is based on the energy
 225 balance between the grains ('internal energy') and the macroscopic sample ('external
 226 energy'). For linking the microscopic and macroscopic properties, the polycrystal has to be
 227 considered as a composite material. Therefore, the Taylor factor has to be based on an energy
 228 relation that is established for composites. In all previous works, the Taylor factors used for
 229 polycrystals were based on the equality of the external and 'the apparent internal energies'
 230 (see its definition in the Appendix), which is valid only in two cases: iso-stress and iso-strain,
 231 or also called Static and Taylor approaches. In other approaches (like the widely used Self-

232 Consistent model), the external and the ‘apparent internal energies’ are not equal, so a
 233 correction is needed. Moreover, there are actually two kinds of Taylor factors; one used for
 234 the strains (equivalent strain macroscopically and crystallographic resolved shear strain
 235 within the grains) and another which is relating the stresses between the two scales
 236 (equivalent stress at the macroscopic level, and crystallographic resolved shear stress in the
 237 grains). The definitions of the two kinds of Taylor factors were established in the Appendix
 238 in such a way that the energy balance for polycrystals is correctly used.

239 We recall first the resulting definition relating the strain quantities:

$$240 \quad M(\text{for strain}) = \frac{\sum_{g=1}^{n_g} \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} (|\dot{\gamma}_s^f| \cdot v_g)}{\bar{\dot{\epsilon}}_c}, \quad (8)$$

241 Here $\dot{\gamma}_s^f$ is the slip rate in the slip system identified with the index ‘s’ for the slip-family ‘f’
 242 (if there is more than one slip system family; frequent in b.c.c. and h.c.p. crystal structures),
 243 whereas, n_f is the number of slip families, and n_s is the number of slip system in a slip
 244 family. n_g is the number of grains and v_g is the relative volume fraction of the grain (so that
 245 the total volume is 1.0). The Taylor factor for converting the stress quantities at the two
 246 scales is:

$$247 \quad M^{(\text{stress})} = \frac{\bar{\sigma}_c}{\lambda \cdot \bar{\tau}_r}, \quad (9)$$

248 where $\bar{\sigma}_c$ is the macroscopic equivalent stress and $\bar{\tau}_r$ is the average resolved shear stress in
 249 the slip systems (see its definition in the Appendix). The λ parameter expresses the ratio of
 250 the ‘external energy’ to the total ‘apparent internal energy’ of the individual grains:

$$251 \quad \lambda = \frac{\underline{\underline{\sigma}}_c : \underline{\underline{\dot{\epsilon}}}_c}{\sum_{g=1}^{n_g} \underline{\underline{\sigma}}_g : \underline{\underline{\dot{\epsilon}}}_g \cdot v_g}. \quad (10)$$

252 Here $\underline{\underline{\sigma}}_c$ and $\underline{\underline{\dot{\epsilon}}}_c$ are the stress and strain rate tensor at the macroscopic level, $\underline{\underline{\sigma}}_g$, $\underline{\underline{\dot{\epsilon}}}_g$ are the
 253 same at grain level. (Note that λ is *not* equal to 1.0 in composite materials, see in Ref. [46].)

254 The Taylor factor for converting the strain quantities at the two scales is:

255

$$M^{(strain)} = \frac{\sum_{g=1}^{n_g} \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} (|\dot{\gamma}_s^f| \cdot \nu_g)}{\dot{\epsilon}} . \quad (11)$$

256

257

258

By doing so, the M factors for strains (Eq. 8) and for stresses (Eq. 9) are always equal. The reason for using one or the other depends on what physical quantity is required to be converted between the macroscopic and microscopic levels.

259

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262

What is needed for the polycrystal simulation is to obtain the values of the microscopic hardening parameters appearing in Eq. (1) (τ_0 , h_c , a_c , τ_{sat}) from the macroscopic ones in Eq. (4) (σ_{00} , h , a and σ_{sat}). Using the Taylor factor defined in Eq. (9) for stresses, the transformation formulas are:

263

$$\tau_0 = \sigma_{00} / M, \quad (12)$$

264

$$\tau_{sat} = \sigma_{sat} / M, \quad (13)$$

265

$$h_c = h / M^2, \quad (14)$$

266

$$a_c = a . \quad (15)$$

267

268

269

First, we examine how to apply these formulas when there is only one slip system family that contributes to the plastic deformation. The Taylor factor can be determined using the polycrystal plasticity code just by doing a single small strain increment, and applying Eq. (9).

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In such a calculation, the value of τ_0 can be arbitrary because M is the ratio of the macroscopic flow stress and the resolved shear stress, while the macroscopic stress is proportional to the resolved shear stress. Having the Taylor factor, all microscopic strain hardening parameters can be obtained by employing Eqs. (12-14), and a full simulation can be done. Nevertheless, before starting a full simulation, it is useful to verify that the macroscopic yield stress is reproduced by the employed Taylor factor. Thus, a single step simulation is required to verify that σ_{00} is actually reproduced by the VPSC simulation. This is not guaranteed because a uniform τ_0 value is used for each grain, while in the real material, the physical quantities are never so ideally homogeneous as in the simulations. Besides, there can be also differences in the grain shapes, or initial texture, both leading to deviations in the Taylor factor of the real material and the simulated one. For all these

281 possible reasons, an adjustment of the Taylor factor might be needed to assure that Eq. (12)
282 becomes valid. This adjustment is simply a multiplication of the simulated Taylor factor by
283 the ratio of the second and the first simulated yield stresses. Once this step is achieved, M and
284 τ_0 are known, and one can determine the other three microscopic parameters using Eqs. (13-
285 15). After this, a full simulation can be performed by the polycrystal code to obtain the
286 macroscopic stress response of the polycrystal. If needed, minor adjustments of the parameter
287 values can still be done to reproduce the experimental measurements better. In the
288 applications presented in this work, only the value of τ_{sat} was needed to be slightly changed
289 to fit the curves well at higher strains. Concerning the self and latent hardening parameters (q_c^{ij}),
290 earlier simulation works have led to general constant values by grouping them into four
291 categories [19], according to the geometrical relation between the slip systems: $q_c^{(1)}=1$ for
292 coplanar slip, $q_c^{(2)}=1.2$ for collinear slip, $q_c^{(3)}=1.4$ for perpendicular slip, and $q_c^{(4)}=1.2$ for all
293 other geometrical situations. These values were used for all simulation cases.

294 On the other hand, assigning the microscopic hardening parameters is a more
295 complex task when several slip system families are active in the material. In this case, the
296 following strategy was adopted in the present work. For the n_f number of families, there are
297 n_f number of τ_0^i and τ_{sat}^i values ($i=1... n_f$). Previous simulation works have led to a set of
298 τ_0^i values, so in the first attempt, they were adopted for calculating the yield stress of the
299 material. In case of difference between the simulated and experimental macroscopic yield
300 stress, the τ_0^i values were scaled proportionally so that the yield stress were the same. This
301 procedure permitted also to obtain a Taylor factor which was then used for calculating the
302 other parameters. Concerning τ_{sat}^i , a single value was assigned for each slip system family,
303 according to Eq. (13).

304 The VPSC polycrystal code in its version developed by Molinari and Toth [47] was
305 employed to predict the Taylor factor (M) as well as to simulate the mechanical response of
306 the polycrystal in the form of stress-strain curves. To constitute the polycrystal, 6000 grain
307 orientations were selected from the measured texture (when it was available), or a random
308 texture was used if the initial texture was not known. For this purpose, the ATEX software
309 [48] was used for the discretization procedure. The strain rate sensitivity index (m) of slip

310 was taken as 0.05 and the α coefficient in the localization law of the self-consistent model
311 was 0.7 (see Molinari and Toth [47] for the details of the VPSC approach used). The flow
312 stress was obtained from the macroscopic stress and strain rate tensors as a work conjugate
313 quantity to the von-Mises equivalent strain rate $\dot{\bar{\epsilon}}_c$:

$$314 \quad \bar{\sigma}_c = (\underline{\underline{\sigma}}_c : \underline{\underline{\dot{\epsilon}}}_c) / \dot{\bar{\epsilon}}_c. \quad (16)$$

315 (Note that here $\bar{\sigma}_c$ is not a von-Mises equivalent stress as the polycrystal is not an isotropic
316 von-Mises material.) Subsequently, the stress-strain curves were plotted using $\bar{\sigma}_c$ as a
317 function of $\bar{\epsilon}_c$.

318

319 **5. Results**

320 The new analytical strain hardening function presented in Eq. (4) was tested for
321 different deformation modes and for materials exhibiting different forms of crystal structures,
322 such as face-centered cubic (FCC), body-centered cubic (BCC) and hexagonal closed packed
323 (HCP). The considered deformation modes were uniaxial tension, compression and torsion
324 testing. The experimental results for evaluating the mechanical response of the materials were
325 adopted from published literature on aluminum [24,49], commercially pure (CP) copper
326 (C110) [50], low carbon steel [22] and titanium (CP-grade 2) [51]. This includes deformation
327 ranging from intermediate to high strain levels. The experimental curves were reproduced in
328 Fig. 1a for aluminum (Al 2024 in T351 state) subjected to uniaxial tension, compression and
329 torsion [49], in Fig. 1b for uniaxial tensile test of copper (C110) [50] as well as for low
330 carbon steel [22]. Fig. 1c presents the stress-strain curve for high torsion strain level for
331 aluminum (Al 1050) [24] and for copper (C110) [50]. Fig. 1d displays the case of HCP-Ti
332 (CP-grade 2) alloys under uniaxial tensile tests at room temperature (RT) and at 300°C [51].

333 For all these above-mentioned cases, the macroscopic parameters were first
334 determined using the presented minimization technique and a comparison of the fitting curves
335 with the experimental ones was accomplished, as discussed in Sec. 5.1. Subsequently, the
336 macroscopic parameters obtained from the analytical approach were transformed into the

337 microscopic ones, i.e., to the grain level, and then simulations were performed using the
338 VPSC code to predict the strain hardening responses, see Sec. 5.2.

339 **5.1. Results obtained from fitting the mechanical response by the phenomenological** 340 **hardening function**

341 Fig. 1 presents the fitted stress-strain responses obtained using the analytical
342 hardening function (Eq. 4) in comparison with the experimental counterparts for the different
343 sets of materials mentioned above under different loading conditions, i.e., tension,
344 compression and torsion. It can be seen that the analytical hardening function (identified as
345 ‘fitted’ in Fig. 1), precisely captures the experimental stress-strain curves. One can appreciate
346 the quality of the fitted stress-strain plots by the analytical hardening function by the fact that
347 we are using only four parameters (i.e., σ_{00} , σ_{sat} , h and a), to reproduce the entire plastic
348 part of the strain hardening curve. Table 1 summarizes the fitted hardening parameters for
349 each of the curves presented in Fig. 1.

350 **5.2. Predicting strain hardening using the VPSC crystal plasticity approach**

351 Figs. 2-5 present the predicted mechanical response and the corresponding strain
352 hardening rate plots obtained by VPSC simulations in comparison with experiments. Results
353 are shown first for the lower strain regime for different strain paths in Fig. 2 for aluminum,
354 and in Fig. 3 for copper and steel. The results for large strain hardening in torsion are
355 presented in Fig. 4 for copper and aluminum. A representative example is also shown for
356 hexagonal crystal structure; for Titanium, see Fig. 5, for two cases: tension parallel (Fig. 5b-
357 c) and perpendicular (Fig. 5d-e) to the rolling direction of the sheet from which the tensile
358 sample was cut. Whenever the experimental initial texture was available (as indicated in
359 Table 2), it was used in the form of a polycrystal with 6000 grains for the VPSC polycrystal
360 simulations; they are also shown in the figures in form of pole figures. When the initial
361 texture was unknown, a random texture was used, also with 6000 grains. One can see that the
362 VPSC simulations reproduce perfectly the experimental curves, just like the
363 phenomenological fitting as shown in Fig. 1.

364 As there is very good agreement between the VPSC-simulated and experimental
365 strain hardening curves, the agreement is also good for their derivatives; $\theta = d\bar{\sigma}/d\bar{\epsilon}$, which
366 constitutes the so-called Kocks-Mecking plot as a function of stress, see in Figs. 2-5. The

367 well-known Stage III and IV hardening stages are indicated for the case of copper and
368 aluminum in Fig. 4.

369

370 **6. Discussion**

371 As the present work has two major parts, we first discuss about the new
372 phenomenological function, and then the crystal plasticity simulations will be examined.
373 Finally, the discussion part will be closed with an evaluation of the applicability conditions
374 for both of these approaches.

375 **6.1. Discussion on the new phenomenological strain hardening function**

376 The new strain hardening function has four parameters, which is a relatively low
377 number with respect to other propositions (for example, the recent modified Ludwigson
378 function [7] has six parameters). In order to obtain the values of the parameters, we
379 established a rapid minimization procedure using about 50 representative points from the
380 experimental curve (Section 3).

381 It is also important to compare the performance of the new proposed
382 phenomenological hardening function to that of existing ones. In this regard, we have carried
383 out such comparisons with two previous propositions: with Chinh et al. [3], and with
384 Lavakumar et al. [7]. Chinh et al. [3] presented a mixed exponential power-law empirical
385 relation for reproducing especially the asymptotic limiting stage (see their equation in Fig.
386 6a). The fitted hardening curves in Fig. 6b correspond to the same experimental curves but
387 obtained by the present phenomenological approach. As can be seen, the agreement is better
388 with the present approach, while both approaches use the same number of parameters (four).

389 Lavakumar et al. [7] proposed a modification to the Ludwigson [1] equation which is
390 a mixed power-law and exponential function (see the function in Fig. 7a). They reproduced
391 satisfactorily the strain hardening behavior of various metallic materials when deformed to a
392 low strain regime (Fig. 7a). We applied our function as well on the same data basis; see the
393 results in Fig. 7b. Closer inspection reveals that our function approaches the experimental
394 curves in better accordance by using only four parameters as compared to six in the modified
395 Ludwigson function.

396 **6.2. Discussion on the crystal plasticity simulations**

397 Tables 3-6 lists the parameters used for predicting the mechanical response using the
398 VPSC approach. They were obtained from the phenomenological analysis by transforming
399 the parameters to the grain level with the help of the Taylor factor. The adjusted Taylor
400 factors are presented in Table 2 together with the simulated Taylor factors (the latter in
401 parenthesis). The difference between the Taylor factors was pointed out in Section 4 above;
402 possibly due to the non-uniform initial strengths of the slip systems in the material, the
403 crystallographic texture (if was not known, so a random texture was used), or the differences
404 in the assumed and experimental grain shapes. Table 2 presents also the values of the λ
405 parameter, which expresses the ratio of the external plastic power to the ‘apparent internal’
406 one (which is the sum of the individual grain-powers). This issue was also examined in the
407 recent work of Sahoo et al. [46] where the strain hardening behavior of two-phase composites
408 were modeled using a plastic power-based composite approach. The range of λ found in the
409 present work is between 1.06 and 1.16, which is quite similar to the range found in Sahoo et
410 al. [46]. λ is always larger than 1.0, meaning that the ‘apparent internal plastic power’
411 calculated within the grains is less than the macroscopic plastic power. As discussed in Sahoo
412 et al. [46], the origin of this unbalance of plastic powers can be attributed to the non-uniform
413 distribution of the stress and strain within the components of the composite, that is, within the
414 grain-interiors of the polycrystal.

415 **6.3. Model limitations**

416 The present modeling is presented for two levels: at the macroscopic level, where the
417 hardening function is totally empirical, and at grain level, for crystal plasticity simulations.
418 The limitations of these two modeling have to be discussed for both the conditions. For the
419 phenomenological case, the function can describe continuous hardening (also continuous
420 softening). As no information is used on the metallurgical state of the metal in the parameter
421 fitting, the parameters are not directly related to a specific material state. Nevertheless, as the
422 proposed function is able to capture the strain hardening response of the material up to large
423 strains (see the torsion example) where significant microstructural evolution is taking place,
424 somehow the parameters are related to those changes. They are: evolution in dislocation
425 density, changes in dislocation cell-size (for alloys showing dislocation cell structures),
426 variation in grain size due to grain fragmentation, or texture evolution due to deformation.

427 On the contrary, for the crystal plasticity modeling, only crystallographic glide was
428 used as a possible deformation mechanism, so the application is more limited. For that case, it

429 is implicitly assumed that the metallurgical state of the alloy does not change during
430 deformation due to phase transformations, twinning or recrystallization. It is designed
431 actually for isothermal conditions and constant strain rate, and not applicable when twinning,
432 phase transformation or dynamic recrystallization is taking place during plastic deformation.

433

434 **7. Summary**

435 The subject of this work is to propose a new strain hardening function with a small
436 number of parameters for use in engineering applications. The new function is based on an
437 earlier crystal plasticity-based hardening function proposed to describe the self and latent
438 hardening of single crystals. It has been successfully applied to several polycrystalline metals
439 with different crystallographic structures and compared with previous approaches. The
440 proposed hardening function has the significant advantage of containing parameters that can
441 be transformed into crystal plasticity parameters, thereby permitting them to be used directly
442 in polycrystal plasticity simulations. This conversion is based on the Taylor factor of the
443 polycrystal. Using these parameters in the VPSC polycrystal model, one can obtain an
444 accurate simulation of the strain hardening curve, like the one obtained by the
445 phenomenological crystal plasticity-based analytical hardening function. It was also shown in
446 this work that there are two kinds of Taylor factors; one for converting the strain and another
447 for the stress quantities between the macroscopic and the grain levels. While they have the
448 same values, their formulas are different; the stress-Taylor factor contains a parameter (λ)
449 which is related to the energy balance between the external and ‘apparent internal plastic
450 power’. This parameter, however, can be readily obtained from the stress and strain quantities
451 computed during the crystal plasticity simulation, and thus the conversion for the stresses is
452 straightforward.

453

454 **8. Acknowledgement**

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458

459

Appendix

460

Taylor factor

461 The Taylor factor is employed to bridge the differences between two scales: the macroscopic
 462 one and the grain level. It can also be used for linking either the strains or stresses. The grain
 463 is a crystal which deforms by slip on several slip systems simultaneously. First, we define the
 464 Taylor factor for a single grain, and then for a polycrystal.

465 Taylor factor for single crystals

466 The slip systems are grouped into families in a grain, according to their common features. We
 467 denote the number of families by n_f and the number of slip systems within one family by n_s
 468 (the f index stands for ‘family’, and the s for slip). The basis for establishing the Taylor
 469 factor is the equality of the ‘internal’ and ‘external’ plastic power in unit volume:

$$470 \quad \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} \tau_s^f \dot{\gamma}_s^f = \sigma_{kl} \dot{\epsilon}_{kl} . \quad (\text{A1})$$

471 Here τ_s^f is the resolved shear stress on a slip system, σ_{kl} is the stress tensor and $\dot{\epsilon}_{kl}$ is the
 472 strain rate tensor. The latter tensorial quantities can be changed into scalars, where $\bar{\dot{\epsilon}}$ is the
 473 von-Mises equivalent strain rate, and $\bar{\sigma}$ is the equivalent stress:

$$474 \quad \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} \tau_s^f \dot{\gamma}_s^f = \bar{\sigma} \cdot \bar{\dot{\epsilon}} . \quad (\text{A2})$$

475 Note that $\bar{\sigma}$ is not the von-Mises equivalent stress (because a crystal is not an isotropic
 476 material); it is the work-conjugate equivalent stress.

477 Using the slip rates, first we define the *average resolved shear stress* $\bar{\tau}_r$:

$$478 \quad \bar{\tau}_r = \frac{\sum_{f=1}^{n_f} \sum_{s=1}^{n_s} \tau_s^f \dot{\gamma}_s^f}{\sum_{f=1}^{n_f} \sum_{s=1}^{n_s} |\dot{\gamma}_s^f|} . \quad (\text{A3})$$

479 Eq. (A2) now becomes:

480
$$\bar{\tau}_r \cdot \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} \|\dot{\gamma}_s^f\| = \bar{\sigma} \cdot \bar{\dot{\epsilon}} \quad . \quad (\text{A4})$$

481 Using this equation, the Taylor factor M_g for a grain ‘g’ can now be defined in two forms,
 482 one for the strains, and another for the stresses:

483
$$M_g^{(strain)} = \frac{\sum_{f=1}^{n_f} \sum_{s=1}^{n_s} \|\dot{\gamma}_s^f\|}{\bar{\dot{\epsilon}}} \quad , \quad M_g^{(stress)} = \frac{\bar{\sigma}}{\bar{\tau}_r} \quad . \quad (\text{A5a,b})$$

484 Note that these two kinds of Taylor factors have the same values. In crystal plasticity
 485 simulations, the Taylor factor can be readily calculated when all quantities needed for its
 486 definition are available. Note that in the work of Mecking et al. [52], Taylor factors were
 487 defined for single crystals, similarly to the present work, designed for strain and stress (Eqs.
 488 5a,b); however, they were defined independently, resulting in disparities in values and
 489 making inconsistencies when they were employed.

490 Taylor factor for polycrystals

491 For polycrystals, the material has to be considered as a composite, made of single
 492 crystals of the same material with number of components equal to the number of grains. The
 493 grains are anisotropic, so the difference between adjacent grains is coming from their
 494 anisotropic mechanical behavior. For a composite material, the equality of the internal and
 495 external powers can only be used as volume integrals (Hill’s lemma), contrary to the case of a
 496 single-phase material (i.e., the single crystal), where the plastic power can be calculated by
 497 the average values of stress and strain rate. First, we write the energy integral for the
 498 polycrystal in the following two forms:

499
$$\sum_{g=1}^{n_g} \int_{V_g} \underline{\underline{\sigma}}_g(\underline{r}) : \underline{\underline{\dot{\epsilon}}}_g(\underline{r}) \cdot dV_g = \int_V \underline{\underline{\sigma}}(\underline{r}) : \underline{\underline{\dot{\epsilon}}}(\underline{r}) \cdot dV \quad . \quad (\text{A6})$$

500 Here, $\underline{\underline{\sigma}}_g(\underline{r})$ and $\underline{\underline{\dot{\epsilon}}}_g(\underline{r})$ are the position dependent stress tensor and strain rate tensors in a
 501 grain ‘g’, while $\underline{\underline{\sigma}}(\underline{r})$, $\underline{\underline{\dot{\epsilon}}}(\underline{r})$ are actually the same, without distinguishing the grains. V_g is
 502 the volume of a grain, and V is the total volume of the polycrystal. According to Hill’s

503 lemma, the volume integral on the right side of Eq. (A6) can be replaced with the
 504 multiplication of the volume averages of the stress and strain rate tensors ($\underline{\underline{\sigma}}_c$, $\underline{\underline{\dot{\epsilon}}}_c$):

$$505 \quad \int_V \underline{\underline{\sigma}}(\underline{r}) : \underline{\underline{\dot{\epsilon}}}(\underline{r}) \cdot dV = \left(\int_V \underline{\underline{\sigma}}(\underline{r}) \cdot dV \right) : \left(\int_V \underline{\underline{\dot{\epsilon}}}(\underline{r}) \cdot dV \right) . \quad (\text{A7})$$

506 These volume integrals can be done grain by grain, so one can write:

$$507 \quad \int_V \underline{\underline{\sigma}}(\underline{r}) \cdot dV = \sum_{g=1}^{n_g} \int_{V_g} \underline{\underline{\sigma}}_g(\underline{r}) \cdot dV_g = \sum_{g=1}^{n_g} \bar{\underline{\underline{\sigma}}}_g \cdot V_g = V \cdot \underline{\underline{\sigma}}_c , \quad (\text{A8})$$

$$508 \quad \int_V \underline{\underline{\dot{\epsilon}}}(\underline{r}) \cdot dV = \sum_{g=1}^{n_g} \int_{V_g} \underline{\underline{\dot{\epsilon}}}_g(\underline{r}) \cdot dV_g = \sum_{g=1}^{n_g} \bar{\underline{\underline{\dot{\epsilon}}}}_g \cdot V_g = V \cdot \underline{\underline{\dot{\epsilon}}}_c , \quad (\text{A9})$$

509 where $\bar{\underline{\underline{\sigma}}}_g$, $\bar{\underline{\underline{\dot{\epsilon}}}}_g$ are the average stress and strain rate tensors within a grain indexed by g ; $\underline{\underline{\sigma}}_c$,
 510 $\underline{\underline{\dot{\epsilon}}}_c$ are the macroscopic stress and strain tensors, respectively and n_g is the number of grains
 511 in the polycrystal. The right-hand side of Eq. (A6) can be called the macroscopic plastic
 512 power (P_c), so the energy balance expressed in Eq. (A6) can be rewritten as:

$$513 \quad \sum_{g=1}^{n_g} \int_{V_g} \underline{\underline{\sigma}}_g(\underline{r}) : \underline{\underline{\dot{\epsilon}}}_g(\underline{r}) \cdot dV_g = V \cdot \underline{\underline{\sigma}}_c : \underline{\underline{\dot{\epsilon}}}_c = P_c . \quad (\text{A10})$$

514 On the other hand, Hill's lemma does not apply to the individual grains within the polycrystal
 515 as a composite, so there is an inequality when one writes the following:

$$516 \quad \sum_{g=1}^{n_g} \int_{V_g} \underline{\underline{\sigma}}_g(\underline{r}) : \underline{\underline{\dot{\epsilon}}}_g(\underline{r}) \cdot dV_g \neq \sum_{g=1}^{n_g} \left(\int_{V_g} \underline{\underline{\sigma}}(\underline{r}) \cdot dV_g \right) : \left(\int_{V_g} \underline{\underline{\dot{\epsilon}}}(\underline{r}) \cdot dV_g \right) = \hat{P} . \quad (\text{A11})$$

517 The right-hand side of this equation will be called hereafter the 'apparent internal plastic
 518 power'; \hat{P} . The two integrals in Eq. (A11) are the average stress and strain values of the
 519 stresses and strain rates within individual grains of the polycrystal, so \hat{P} can be written as:

$$520 \quad \hat{P} = \sum_{g=1}^{n_g} \bar{\underline{\underline{\sigma}}}_g : \bar{\underline{\underline{\dot{\epsilon}}}}_g \cdot V_g . \quad (\text{A12})$$

521 In a polycrystal plasticity modeling, both P_c and \hat{P} can be calculated, so by introducing a
 522 scalar parameter (λ) between them, we can write:

$$523 \quad \lambda \hat{P} = P_c . \quad (\text{A13})$$

524 The value of λ is a measure of the deviation between the ‘external plastic power’ and the
 525 ‘apparent internal plastic power’:

$$526 \quad \lambda = \frac{\underline{\underline{\sigma}}_c : \underline{\underline{\dot{\epsilon}}}_c}{\sum_{g=1}^{n_g} \bar{\underline{\underline{\sigma}}}_g : \bar{\underline{\underline{\dot{\epsilon}}}}_g \cdot v_g} . \quad (\text{A14})$$

527 Here v_g is the volume fraction of a grain: $v_g = V_g / V$. As λ is defined by Eq. (A14), and all
 528 quantities are available to calculate its value from a polycrystal plasticity code, the value of λ
 529 can be calculated by Eq. (A14).

530 Now the apparent plastic power \hat{P} , defined by (A12), is rewritten for the polycrystal using
 531 the resolved shear stresses and resolved shear strain rates:

$$532 \quad \hat{P} = V \cdot \sum_g^{n_g} \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} (\tau_s^f \cdot \dot{\gamma}_s^f \cdot v_g) . \quad (\text{A15})$$

533 This is done in order to replace the tensorial quantities with scalar ones. Similar change can
 534 be done also for the external plastic power, P_c . Using its expression given by the right-hand
 535 side of Eq. (A10), we write:

$$536 \quad P_c = V \cdot \underline{\underline{\sigma}}_c : \underline{\underline{\dot{\epsilon}}}_c = V \cdot \bar{\underline{\underline{\sigma}}}_c \cdot \bar{\underline{\underline{\dot{\epsilon}}}}_c , \quad (\text{A16})$$

537 where $\bar{\underline{\underline{\dot{\epsilon}}}}_c$ is the von-Mises equivalent strain rate, and $\bar{\underline{\underline{\sigma}}}_c$ is the work-conjugate equivalent
 538 stress, defined by Eq. (A16):

$$539 \quad \bar{\underline{\underline{\sigma}}}_c = \frac{\underline{\underline{\sigma}}_c : \underline{\underline{\dot{\epsilon}}}_c}{\dot{\epsilon}_c} , \quad (\text{A17})$$

540 Then Eq. (A13) can be written as:

541
$$\lambda \cdot \sum_g^{n_g} \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} (\tau_s^f \cdot \dot{\gamma}_s^f \cdot \nu_g) = \bar{\sigma}_c \cdot \bar{\dot{\epsilon}}_c . \quad (\text{A18})$$

542 Similar to the case of single crystal, the expression of the average resolved shear stress $\bar{\tau}_r$ for
 543 a polycrystal becomes:

544
$$\bar{\tau}_r = \frac{\sum_{g=1}^{n_g} \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} (\tau_s^f \cdot \dot{\gamma}_s^f \cdot \nu_g)}{\sum_{g=1}^{n_g} \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} (|\dot{\gamma}_s^f| \cdot \nu_g)} . \quad (\text{A19})$$

545 Eq. (A18) is written then:

546
$$\lambda \cdot \bar{\tau}_r \cdot \sum_{g=1}^{n_g} \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} (|\dot{\gamma}_s^f| \cdot \nu_g) = \bar{\sigma}_c \cdot \bar{\dot{\epsilon}}_c . \quad (\text{A20})$$

547 From this, the Taylor factor M for polycrystals is calculated in its two forms as:

548
$$M^{(strain)} = \frac{\sum_{g=1}^{n_g} \sum_{f=1}^{n_f} \sum_{s=1}^{n_s} (|\dot{\gamma}_s^f| \cdot \nu_g)}{\bar{\dot{\epsilon}}_c} , \quad M^{(stress)} = \frac{\bar{\sigma}_c}{\lambda \cdot \bar{\tau}_r} , \quad (\text{A21a,b})$$

549 where λ is computed from Eq. (A14). Note that the values of these two Taylor factors are the
 550 same. These definitions can be used in any polycrystal model as there was no implied
 551 assumption in its definition on the uniformity of strain (Taylor model), or the stress (Static
 552 model), or heterogeneous deformation (Self-consistent model, where both stress and strain in
 553 a grain can be different from the macroscopic ones).

Figure Captions:

Fig. 1. Fitted stress-strain response obtained from analytical phenomenological hardening curve, compared to measurements.

Fig. 2. VPSC simulation results for aluminum (Al 2024) in comparison with experimental measurements for (a) stress-strain response and (b) strain hardening rate.

Fig. 3. Initial input texture used for VPSC simulation for (a) Steel and (b) Copper (C110). Comparative plots of both the experimental and predicted (c) stress-strain response and (d) strain hardening rate behavior of both the tested specimens obtained from the VPSC simulation.

Fig. 4. Initial input texture used for VPSC simulation for (a) Aluminum (Al 1050) and (b) Copper (C110). Comparative plots of both the experimental and predicted (c) stress-strain response and (d-e) strain hardening rate behavior of both the tested specimens obtained from the VPSC simulation.

Fig. 5. Initial input texture used for VPSC simulation for (a) rolled titanium (CP-grade 2) sample similar to the published literature (Orozco-Caballero et al., 2018).

(b-e) Comparative plots of both the experimental and predicted stress-strain response and strain hardening rate behavior obtained from the VPSC simulation for tension parallel and perpendicular to the rolling direction at room temperature and 300°C.

Fig. 6. Comparison of the strain hardening plots between (a) the function of Chinh et al. (2004) and (b) the proposed analytical phenomenological function.

Fig. 7. Comparison of the strain hardening plots between (a) the modified Ludwigs function (Lavakumar et al. (2021)), and (b) the proposed analytical phenomenological function.

Table Captions:

Table 1. The hardening parameters obtained by fitting the new phenomenological hardening law for different materials and testing conditions.

Table 2. The predicted and the adjusted values of the Taylor factor for different materials, the λ parameter and the test conditions obtained by VPSC simulation.

Table 3. The hardening parameters used in the VPSC simulations to fit the phenomenological hardening law corresponding to different materials and test conditions.

Table 4. The hardening parameters used in the VPSC simulation to fit the phenomenological hardening law corresponding to steel.

Table 5. The hardening parameters for HCP-Ti tensile testing used in VPSC simulations.

Table 6. Initial Reference Resolved Shear Stresses for hexagonal slip system families, in [MPa].

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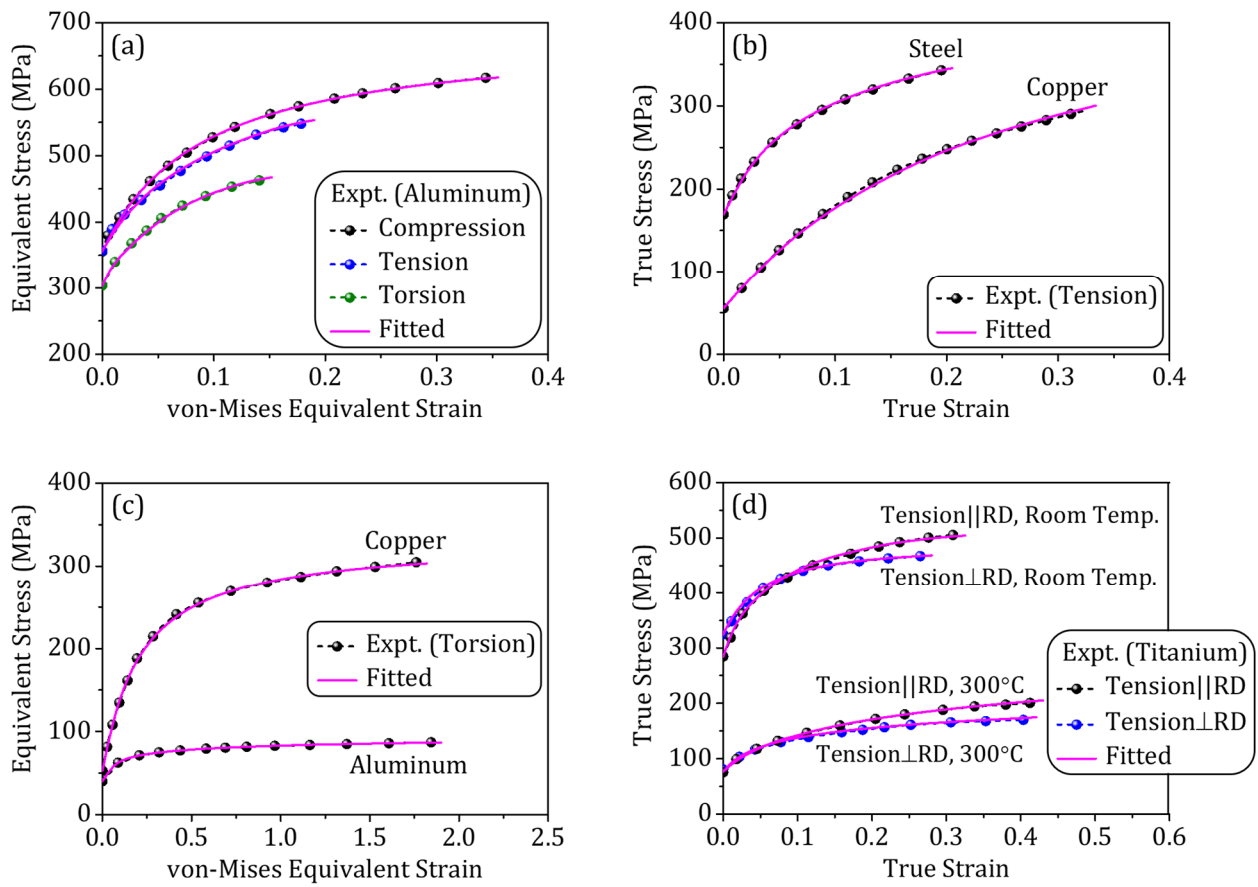


Fig. 1. Fitted stress-strain response obtained from analytical phenomenological hardening curve, compared to measurements.

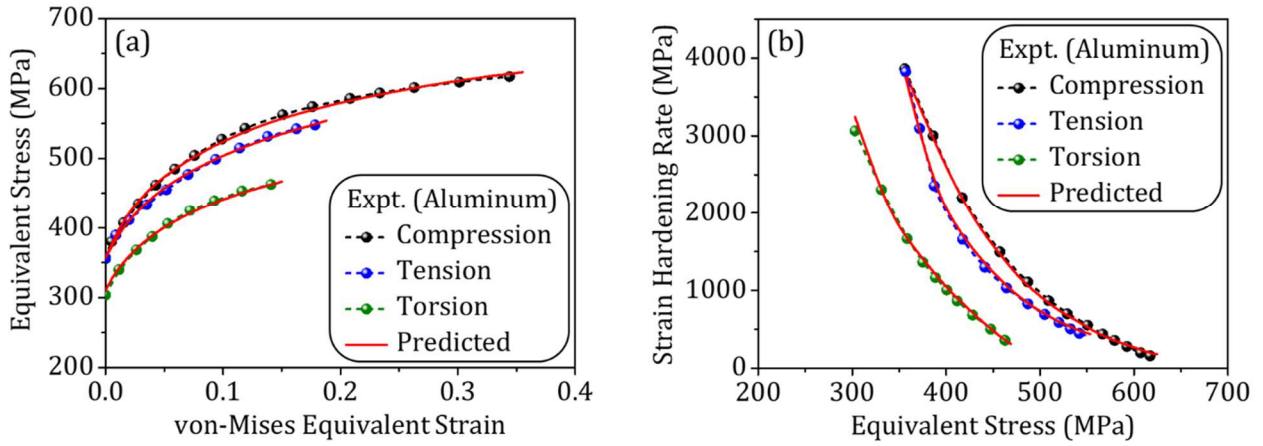


Fig. 2. VPSC simulation results for aluminum (Al 2024) in comparison with experimental measurements for (a) stress-strain response and (b) strain hardening rate.

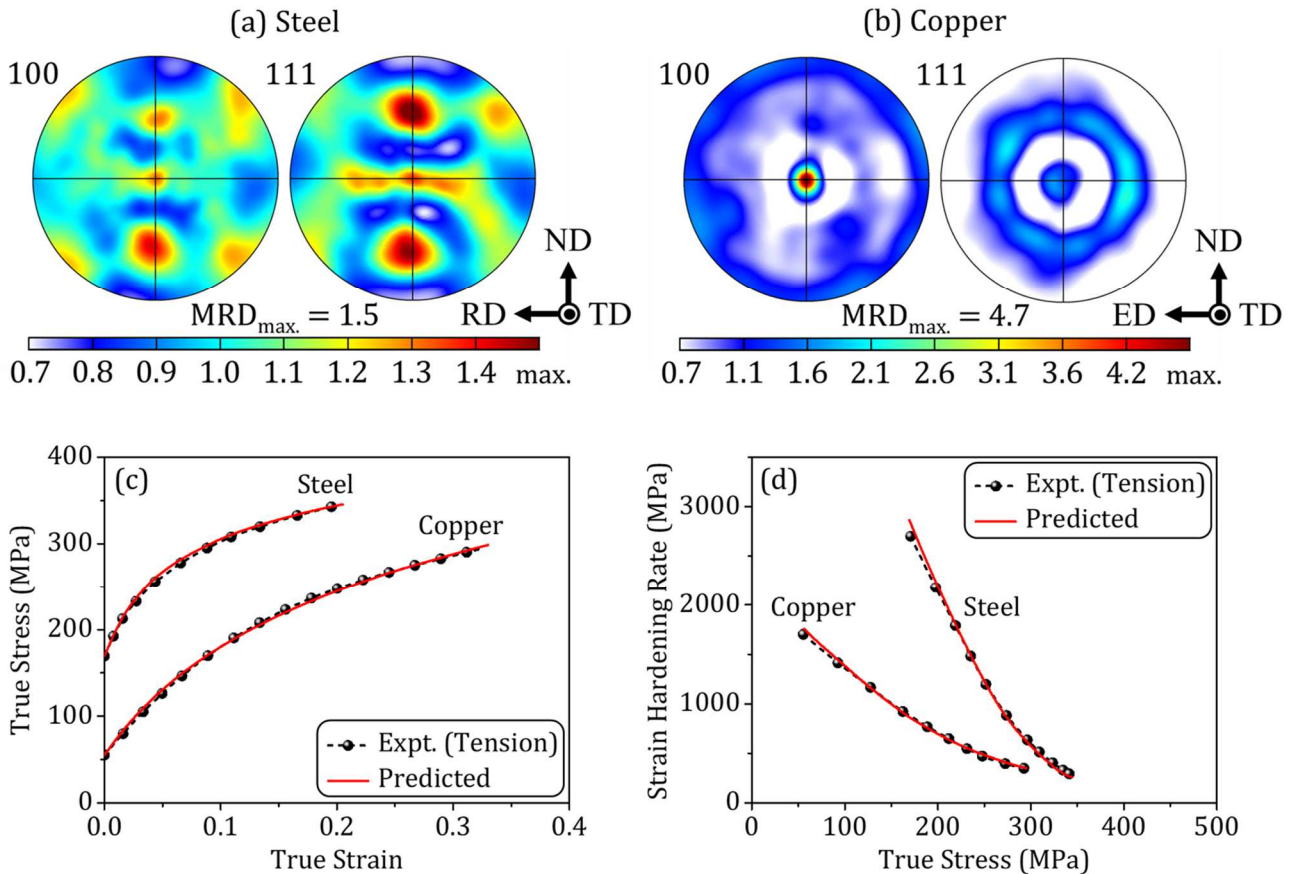


Fig. 3. Initial input texture used for VPSC simulation for (a) Steel and (b) Copper (C110). Comparative plots of both the experimental and predicted (c) stress-strain response and (d) strain hardening rate behavior of both the tested specimens obtained from the VPSC simulation.

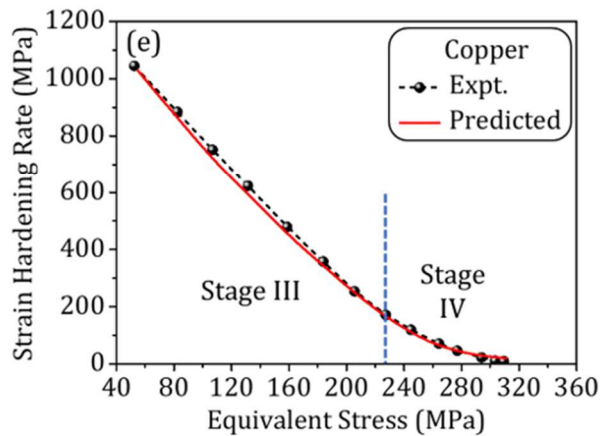
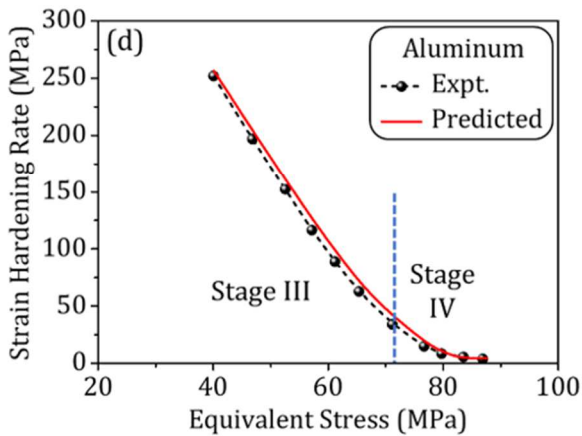
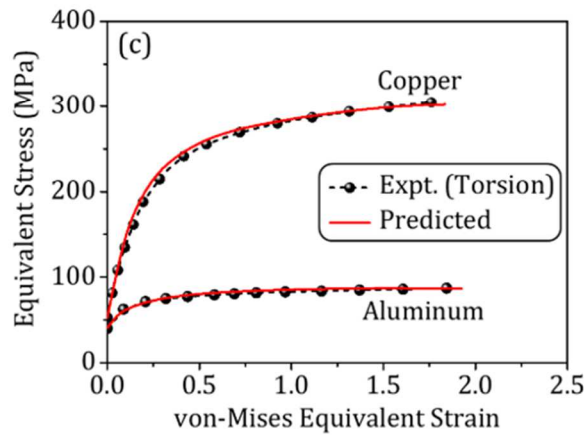
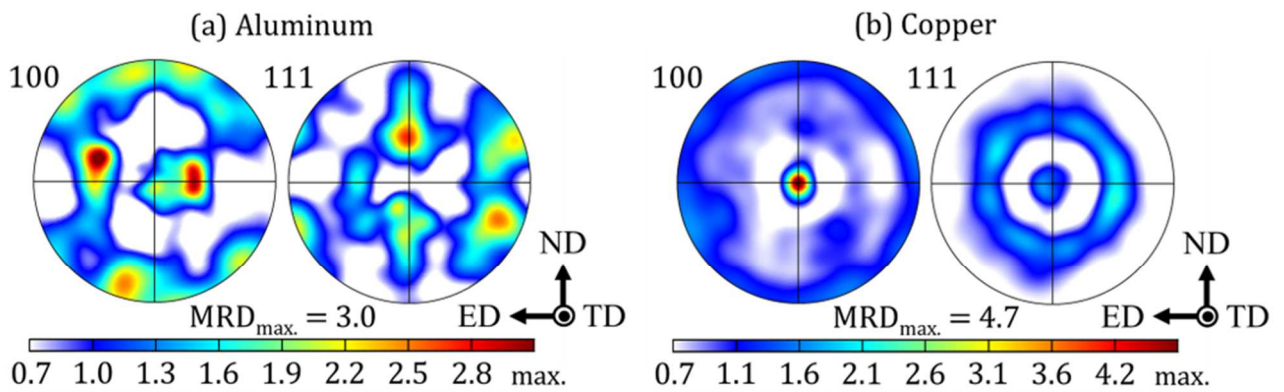


Fig. 4. Initial input texture used for VPSC simulation for (a) Aluminum (Al 1050) and (b) Copper (C110). Comparative plots of both the experimental and predicted (c) stress-strain response and (d-e) strain hardening rate behavior of both the tested specimens obtained from the VPSC simulation.

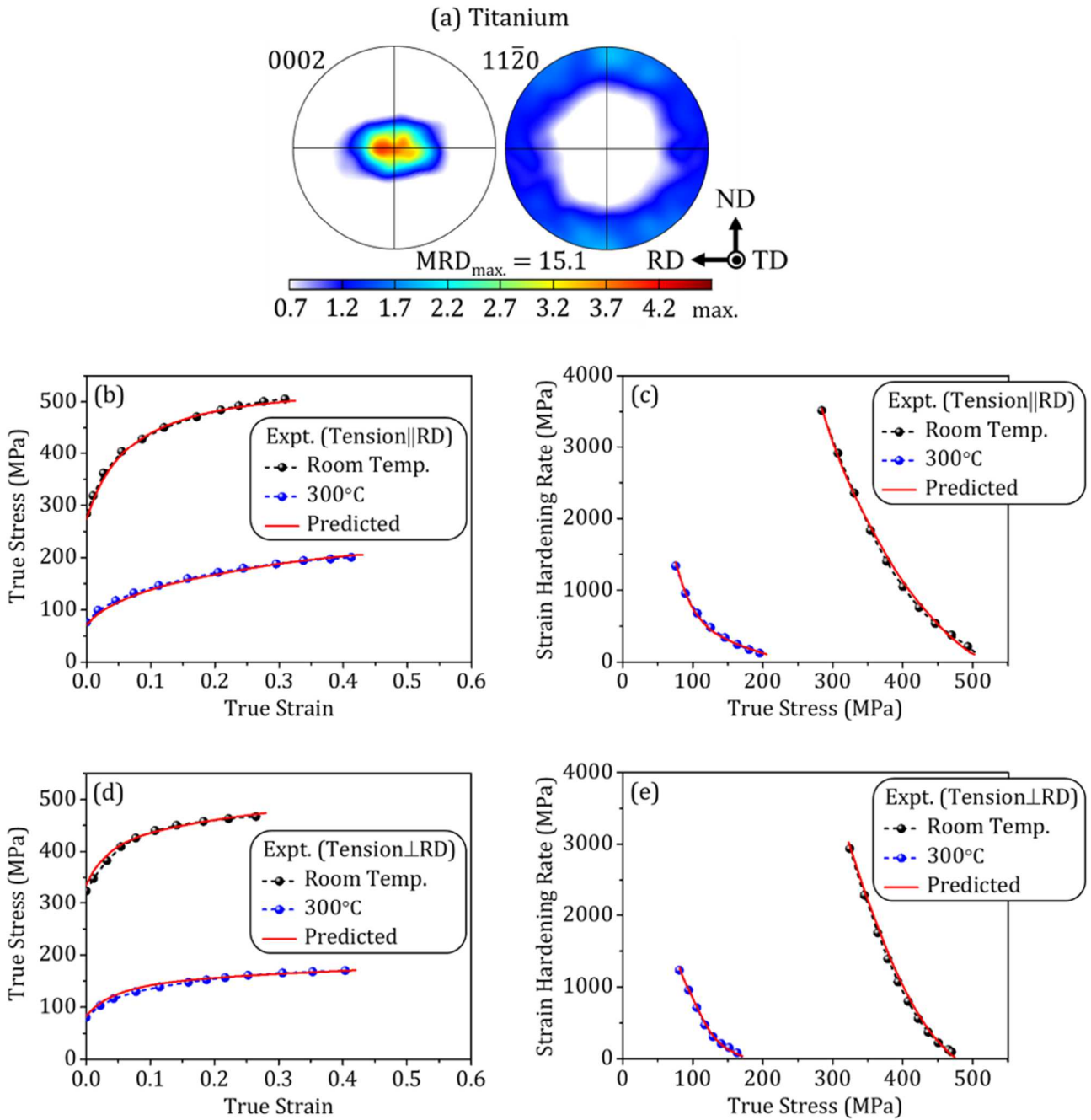
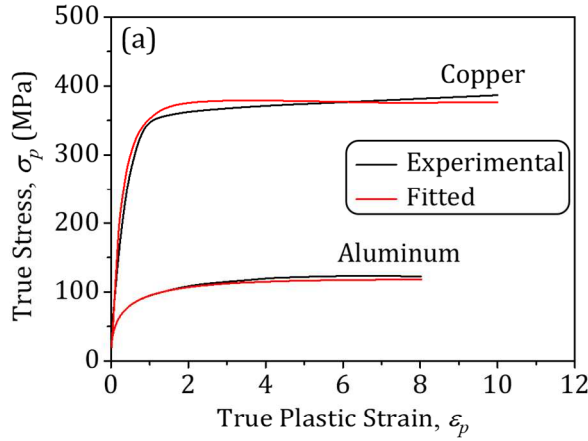


Fig. 5. Initial input texture used for VPSC simulation for (a) rolled titanium (CP-grade 2) sample similar to the published literature (Orozco-Caballero et al., 2018).

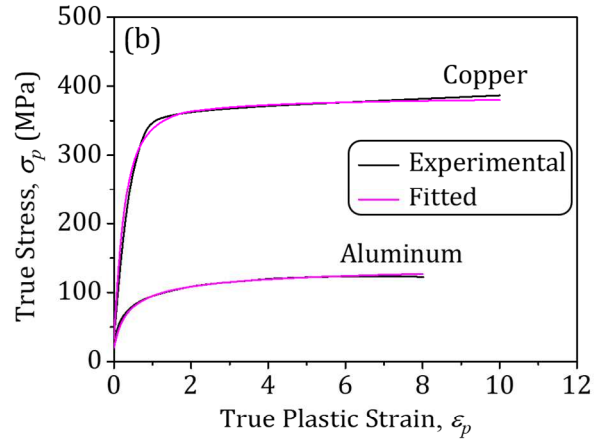
(b-e) Comparative plots of both the experimental and predicted stress-strain response and strain hardening rate behavior obtained from the VPSC simulation for tension parallel and perpendicular to the rolling direction at room temperature and 300°C.



Exponential power-law relationship
(Chinh et al., 2004):

$$\sigma = \sigma_0 + \sigma_1 \left[1 - \exp\left(-\frac{\varepsilon^n}{\varepsilon_c}\right) \right]$$

Parameters used: $\sigma_0, \sigma_1, \varepsilon_c, n$

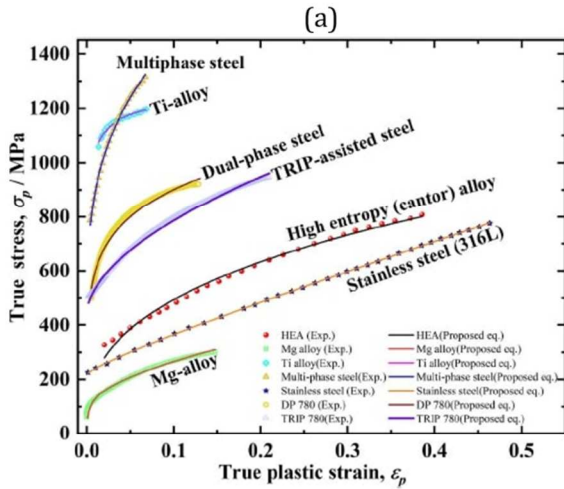


Proposed analytical equation:

$$\sigma_0(\bar{\varepsilon}) = \sigma_{sat} - \sigma_{sat} \left[\left(\frac{h(a-1)}{\sigma_{sat}} \right) \bar{\varepsilon} + \left(1 - \frac{\sigma_{00}}{\sigma_{sat}} \right)^{1-a} \right]^{\frac{1}{1-a}}$$

Parameters used: $\sigma_{00}, \sigma_{sat}, h, a$

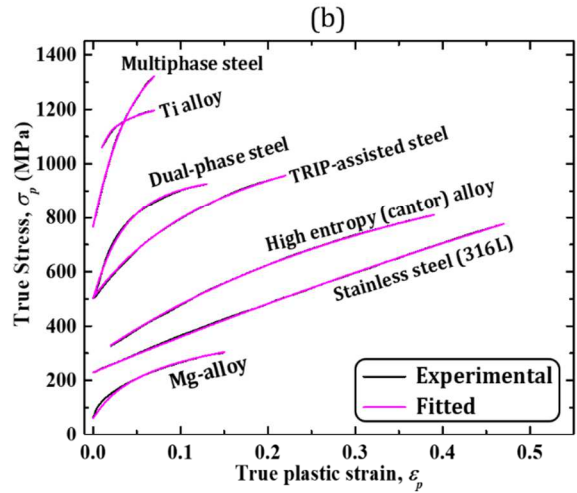
Fig. 6. Comparison of the strain hardening plots between (a) the function of Chinh et al. (2004) and (b) the proposed analytical phenomenological function.



Modified Ludwigungson equation
(Lavakumar et al., 2021):

$$\sigma = K_1 \varepsilon_p^{n_1} + \exp(K_2 + n_2 \varepsilon_p) - \exp(K_3 + n_3 \varepsilon_p)$$

Parameters used: $K_1, n_1, K_2, n_2, K_3, n_3$



Proposed analytical equation:

$$\sigma_0(\bar{\varepsilon}) = \sigma_{sat} - \sigma_{sat} \left[\left(\frac{h(a-1)}{\sigma_{sat}} \right) \bar{\varepsilon} + \left(1 - \frac{\sigma_{00}}{\sigma_{sat}} \right)^{1-a} \right]^{\frac{1}{1-a}}$$

Parameters used: $\sigma_{00}, \sigma_{sat}, h, a$

Fig. 7. Comparison of the strain hardening plots between (a) the modified Ludwigungson function (Lavakumar et al. (2021)), and (b) the proposed analytical phenomenological function.

Table 1. The hardening parameters obtained by fitting the new phenomenological hardening law for different materials and testing conditions.

Figure	Material, Testing	Yield strength (σ_{00}) [MPa]	Saturation stress (σ_{sat}) [MPa]	Hardening coefficient (h) [MPa]	Hardening exponent (a)
Fig. 1a	Aluminium Compression at RT	355	995	30940	4.90
	Aluminium Tension at RT	357	955	31221	4.90
	Aluminium Torsion at RT	300	879	21953	4.90
Fig. 1b	Copper Tension at RT	56	695	2127	3.10
	Low Carbon Steel Tension at RT	170	640	13998	4.89
Fig. 1c	Copper Torsion at RT	52	390	1839	3.10
	Aluminium Torsion at RT	42	98	3268	4.52
Fig. 1d	Titanium Tension RD, RT	284	528	12578	1.61
	Titanium Tension ⊥ RD, RT	324	485	16317	1.61
	Titanium Tension RD 300°C	76	390	2350	4.08
	Titanium Tension ⊥ RD 300°C	80	305	2866	4.08

Table 2. The predicted and the adjusted values of the Taylor factor for different materials, the λ parameter and the test conditions obtained by VPSC simulation.

Figure	Material, testing, initial texture	{VPSC} adjusted Taylor factor	λ
Fig. 2	Aluminium Compression at RT Random texture	{2.47} 2.22	1.15
	Aluminium Tension at RT Random texture	{2.49} 2.23	1.14
	Aluminium Torsion at RT Random texture	{2.39} 1.87	1.12
Fig. 3	Copper Tension at RT Measured texture	{2.43} 2.24	1.15
	Low Carbon Steel Tension at RT Measured texture	{2.34} 2.05	1.14
Fig. 4	Copper Torsion at RT Measured texture	{2.41} 2.08	1.13
	Aluminium Torsion at RT Measured texture	{2.42} 2.1	1.11
Fig. 5	Titanium Tension RD, RT Measured texture	{2.20} 2.59	1.09
	Titanium Tension ⊥ RD, RT Measured texture	{2.26} 2.95	1.2
	Titanium Tension RD, 300°C Measured texture	{2.25} 2.11	1.06
	Titanium Tension ⊥ RD, 300°C Measured texture	{2.38} 2.22	1.14

Table 3. The hardening parameters used in the VPSC simulations to fit the phenomenological hardening law corresponding to different materials and test conditions.

Figure	Material, testing, initial texture	Taylor Factor	τ_0 for $\{111\}\langle 110\rangle$ [MPa]	Saturation stress (τ_{sat}) [MPa]	Hardening coefficient (h_c) [MPa]	Hardening exponent (a_c)
Fig. 2	Aluminium Compression at RT Random texture	2.22	160	421	6278	4.90
	Aluminium Tension at RT Random texture	2.23	160	394	6278	4.90
	Aluminium Torsion at RT Random texture	1.87	160	388	6278	4.90
Fig. 3	Copper Tension at RT Measured texture	2.24	25	253	424	3.10
Fig. 4	Copper Torsion at RT Measured texture	2.08	25	190	424	3.10
	Aluminium Torsion at RT Measured texture	2.1	20	43	706	4.52

Table 4. The hardening parameters used in the VPSC simulation to fit the phenomenological hardening law corresponding to steel.

Figure	Material, testing, initial texture	Taylor Factor	τ_0 for $\{110\}\langle 111\rangle$ [MPa]	τ_0 for $\{112\}\langle 111\rangle$ [MPa]	Saturation stress (τ_{sat}) [MPa]	Hardening coefficient (h_c) [MPa]	Hardening exponent (a_c)
Fig. 3	Steel Tension at RT Measured texture	2.05	83	79	299	3331	4.89

Table 5. The hardening parameters for HCP-Ti tensile testing used in VPSC simulations.

Figures	Material, testing, initial texture	Saturation stress (τ_{sat}) (MPa)	Hardening coefficient (h_c) (MPa)	Hardening exponent (a_c)
Fig. 5	Titanium Tension RD, RT Measured texture	317	1875	1.61
	Titanium Tension ⊥ RD, RT Measured texture	286	1875	1.61
	Titanium Tension RD, 300°C Measured texture	180	528	4.08
	Titanium Tension ⊥ RD, 300°C Measured texture	153	528	4.08

Table 6. Initial Reference Resolved Shear Stresses for hexagonal slip system families, in [MPa].

	Prismatic	Basal	Pyramidal <a>	Pyramidal <c+a>
RT	110	179	142	243
300°C	36	36	36	254