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Microstructure scale modelling of the WC and Co phases plastic behaviour in the WC-Co composite with different cobalt contents and for different temperatures. Comparison of the Drucker-Prager and Mises models

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34 Cobalt (Co) binder and hard-brittle carbide (WC) grains [3–5] which is sintered around 1400°C [2].
35 Thus, the mechanical properties depend on many parameters such as the increase in hardness as the
36 WC grain size and the weight percentage of Co (wt.%) decrease. In general, the WC grain size of
37 ranges from 0.5 to 2 μm with a cobalt weight percentage ranging from 5 to 16% [6]. However, for
38 some specific applications, such as the machining of metals or hard superalloys for example, the
39 percentage by weight of cobalt is most of the time lower than 10%, according to the literature.

40 Many researches and development works mainly experimental have been conducted on the whole the
41 supply chain of the initial WC-Co tool, from their manufacturing process to their breakdown (the end
42 of their lifetime) [7–9]. Several authors have been particularly interested in behaviour of these WC-Co
43 tools under extreme thermal and mechanical loadings [10–12] encountered in machining. For instance,
44 in the investigation led by Davies *et al.* [13], a temperature of 1000°C along the tool-chip contact was
45 achieved due to an intense friction during the machining of the AISI 1045 steel with a cutting speed of
46 605 $\text{m} \cdot \text{min}^{-1}$ and uncut chip thicknesses of 133 μm . In addition, a temperature gradient in the tool
47 was observed especially from the tool tip to the end of the tool-chip contact and also to the center of
48 the tool where the temperature decreases. Many studies have been carried out on the WC-Co
49 behaviour under large range of temperatures between 25 °C and 1000°C. Ueda *et al.* [11] and Emani
50 *et al.* [14] identified three main temperature ranges where the WC/Co carbide tool exhibits different
51 mechanical behaviours. In the range of 25 °C to 527 °C, Mari [15] observed a brittle and elastic WC-
52 Co behaviour explained by the multiple intersections of stacking faults in the cobalt phase blocking
53 the crystal lattice and inhibiting any movement [16]. From 527 °C to 827 °C, an increase of toughness
54 induced by the softening of cobalt with a limited plastic deformation were observed. For temperatures
55 over 827 °C and below 1000°C, the sliding of the WC grain boundaries is one of the mechanisms
56 involving the softening of WC-Co subjected to larger plastic deformations.

57 In parallel with the experimental studies, the numerical simulation approach was also used to analyse
58 the contribution of each phase in the mechanical behaviour of WC-Co at the microstructure scale. This
59 work can be classified into two groups. The first group concerns the simulation of damaged WC-Co
60 [17, 18]. The second one models the elasto-plastic behaviour of WC-Co prior to damage and on which
61 the present study focuses. Without being exhaustive, some significant studies of this second group are
62 recalled in the following, before introducing the subject of this paper.

63 In 1972 Jaensson *et al.* [19] proposed the first finite element simulations to compute the Young's
64 modulus and Poisson's ratio of the WC-Co composite from 2D representative volume elements (RVE).
65 These RVE were created from realistic microstructures composed of 20-30 carbides grains. Each
66 phase has an elastic behaviour. A good agreement between experimental data and simulation results
67 for different percentages of cobalt (1-30wt.%) was found. Thereafter, this work was extended by
68 Sundstrom [20] to simulate the elasto-plastic behaviour of the composite in compression. Elasto-

69 plastic and elastic models were used for cobalt and WC, respectively. The results revealed that the
70 plastic deformations are possible in the cobalt binder despite the presence of WC hard matrix phase. In
71 addition, local plastic strains can reach twice times the value of the effective plastic strain. Twenty
72 years later, Poech *et al.* [21] evaluated the possible impact of the microstructural parameters such as
73 the shape and arrangement of the binder phase on the elasto-plastic behaviour of the WC-Co. The
74 results show that these parameters have a slight influence on the strain-stress curves. The authors
75 analysed the effect of the mesh geometry, mesh density and model size on the results. They showed
76 that the yield stress of the composite decreases to a constant value for the densest meshes. Later, and
77 thanks to more computing power, Sadowski *et al.* [22] performed numerical simulations on several
78 sizes of representative surface features (RSE) or 2D RVE much larger than those used in previous
79 works. They contain many grains (>120 grains for a RSE size of $10 \times 10 \mu\text{m}$) and are created from real
80 microstructures. The best fit to the experimental data was obtained with the largest RSE ($40 \times 40 \mu\text{m}$)
81 under conditions of generalized plane strain. In a continuation of previous work, Chen *et al.* [23]
82 proposed a statistical method for defining the minimum size of the 2D representative volume element
83 of the WC-Co alloy and found that the RVE for a plastic study must be larger than that for an elastic
84 study. The mean value of each parameter considered as the effective elastic constants or the
85 anisotropic parameter converge from a RVE size of $30 \times 30 \mu\text{m}$ but their respective standard deviation
86 decreases further. From the obtained results, a RVE size of $40 \times 40 \mu\text{m}$ is recommended by the authors.
87 However, in the previous studies, the compression of the WC-Co is limited to strains lower than 0.6%.
88 According to Poech *et al.* [21], after the initial plasticity of the composite, it is necessary to consider
89 both the plastic and damage processes in the carbide phase. Tkalich *et al.* [24] proposed to simulate
90 only the plasticity of the carbide with Drucker-Prager's isotropic model. This model is able to
91 reproduce the difference in strength of the WC material under compression and tension. In their work,
92 the elasto-plastic behaviour of the composite was simulated using a 2D RVE based on realistic
93 microstructures and under generalized strain plane conditions. The decrease in strain rate after initial
94 plasticity, often observed in the literature, is well reproduced. The authors then extended their model
95 in another study [25] to an idealized 3D RVE created from an algorithm based on Voronoi cells.
96 Several complex mechanical loads were applied on this RVE to estimate the shape of the initial
97 elasticity surface of different WC-Co composites which is similar to a Drucker-Prager surface with a
98 cap. However, for all numerical studies presented in this introduction, the simulations were performed
99 at room temperature. As mentioned above, the WC-Co cutting tool is subjected to high temperatures
100 up to 1000°C , which can change the mechanical behaviour of the composite. Recently, Faksa *et al.*
101 [26] simulated the elasto-plastic behaviour of the WC-6wt.%Co composite in compression for the
102 temperature range of 20 to 900°C using a 2D RVE. Due to a lack of data, the pure Co was substituted
103 by a cobalt alloy. The first results of the study showed that only the elasto-plastic behaviour of Co is
104 insufficient to represent the plasticity of the composite for strains above 0.6% in the case of elastic
105 WC behaviour. Therefore, a plastic behaviour was assumed for the WC phase. The stress-strain curves

106 of the WC are inversely reconstructed from the composite behaviour. However, this study is limited to
107 WC-6wt.%Co composite.

108 This state of the art reveals the need to clarify the different behaviours of the tungsten carbide phase
109 used in the literature. Although data on the elasto-plastic behaviour of WC are scarce, it is possible to
110 identify it by an inverse approach similar to that adopted by Faksa *et al.* [26] with a pure cobalt phase.
111 Finally, a finite element analysis of the elasto-plastic behaviour of WC-Co hard metal at the
112 microstructural scale needs to be developed for different temperatures and cobalt contents. These
113 shortcomings, mentioned above, are the subject of the present study.

114 This paper is structured as follow:

115 In Section 2, the elasto-plastic models to simulate the behaviour of the cobalt and WC phases are
116 presented. For the carbide phase, the von Mises and Drucker Prager criteria used in the work of
117 Tkalich *et al.* [24, 25] are proposed but only at room temperature. Then, in Section 3, an algorithm to
118 generate idealized WC-Co microstructures is described. The advantage of this strategy is to control the
119 cobalt content and the number of WC grains. In Section 4, a study is carried out to establish the
120 number of WC grains necessary to build an RVE for the elasto-plastic behaviour of the composite at
121 room temperature. Then, in Section 5, a temperature-dependent hardening law for the WC phase is
122 determined from the behaviour of the composite WC-6 wt.%Co and the pure cobalt. The model is
123 tested for a WC-10.5wt.% Co composite in uniaxial compression and the results are compared with
124 literature data. Finally, a comparison between the von Mises and Drucker-Prager criteria applied to the
125 WC phase is carried out. Some conclusions from this study are then given.

126 **2. Modelling of the Co and WC phases behaviour**

127 The modelling of the WC-Co elastoplastic behaviour at the microstructure scale requires suitable
128 behaviour models dedicated to the Co and WC phases.

129 **2.1 Elastic behaviour**

130 The ductile phase of the cobalt is polycrystalline with a crystallite size of 3 times larger than that of
131 the WC grains [27]. Its elastic behaviour is assumed to be isotropic. The Young's modulus and thermal
132 expansion as a function of the temperature are taken from data given by Betteridge in [28] and Fine
133 and Ellis in [29], see Figure 1. The Poisson's ratio is taken equal to 0.31 from the work of Poech *et al.*
134 [21] since Teppernegg *et al.* [30] have shown its insensitivity to the temperature evolution.

135 The WC phase consists of several grains. Each grain has a transversely isotropic elastic behaviour due
136 to its hexagonal crystal structure. However, most studies in literature [31, 32] using microstructural
137 simulations of the WC-Co composite assume that each grain has the isotropic elastic behaviour of the
138 polycrystal WC. This hypothesis is also chosen in the present study. The Young's modulus and

139 thermal expansion as a function of temperature are given in Figure 2 and are taken from [21] and [33].
 140 The Poisson's ratio taken insensitive to the temperature is equal to 0.194 [21].

141 2.2 Plastic Model

142 In this section, the elasto-plastic model for the cobalt is presented. As mentioned in Introduction, in
 143 the models, the plasticity of the composite is mainly due to the plasticity of the cobalt phase, whereas
 144 the WC phase is often considered as an elastic medium. However, some authors [24, 26] assumed an
 145 elasto-plastic behaviour of the WC phase justified in the literature by the presence of slip marks
 146 observed in WC grains [34–36] or by a disorientation of WC grains observed in a deformed WC-
 147 6wt.%Co sample indicating some extension of plastic deformation [26]. Two elasto-plastic models of
 148 the WC used by these authors are also introduced in the following and will be compared and discussed
 149 later in this paper.

150 2.2.1 von Mises criterion for Cobalt and WC phases

151 The von Mises criterion usually used for metallic materials is adopted here for the cobalt phase. In a
 152 first approach, von Mises criterion can be transposed to the carbide phase. Faksa et al. [26] also
 153 adopted a plastic behaviour for both phases in ABAQUS software [37] that is based on the von Mises
 154 criterion. In the elasto-plastic regime of a phase “*i*” (*i* = carbide phase WC , cobalt phase C_o), von
 155 Mises criterion is chosen to describe its yield surface which is defined by:

$$156 \quad f_i(\boldsymbol{\sigma}, p) = J_2(\boldsymbol{\sigma}) - (R_i + Y_i(p)) \quad (1)$$

157 with $J_2(\boldsymbol{\sigma}) = \sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}}$ the von Mises stress computed operator from $\mathbf{s} = \boldsymbol{\sigma} - \frac{1}{3} \text{trace}(\boldsymbol{\sigma})$ the deviatoric
 158 part of the stress tensor $\boldsymbol{\sigma}$. Bold letters are used to denote vectors and tensors. R_i and $Y_i(p)$,
 159 respectively, the yield stress and the isotropic hardening with p is the accumulated plastic strain which
 160 is defined by:

$$161 \quad p = \int_0^t \sqrt{\frac{2}{3} \dot{\boldsymbol{\epsilon}}^p : \dot{\boldsymbol{\epsilon}}^p} dt \quad (2)$$

162 with, $\dot{\boldsymbol{\epsilon}}^p$ the plastic strain rate tensor and “:” the double contraction operator.

163 $\dot{\boldsymbol{\epsilon}}^p$ is calculated from the following associate flow rule:

$$164 \quad \dot{\boldsymbol{\epsilon}}^p = \dot{\lambda} \frac{\partial g_i}{\partial \boldsymbol{\sigma}} \quad (3)$$

166 with $\dot{\lambda}$, the plastic multiplier and g_i flow potential defined which is equal to f_i from Equation (1).

167 The term $R_i + Y_i(p)$ describes a plastic stress-strain curve that can be obtained from a tensile or
 168 compression test. For the Co phase, these curves were measured in compression by Park *et al.* [38] for
 169 different temperatures, see Figure 3, and then described by a series of points written in a table in the
 170 ABAQUS software. The intermediate data between two points are calculated by linear interpolation.
 171 In the case of WC ($i = WC$), the term $R_{WC} + Y_{WC}(p)$ is taken from Tkalich *et al.* [24] where the
 172 isotropic hardening $Y_{WC}(p)$ is defined as follows:

$$173 \quad Y_{WC}(p) = Q_{WC}[1 - \exp(-b_{WC}p)] \quad (4)$$

174 where Q_{WC} and b_{WC} are the hardening constants. The values of parameters $R_{WC} = 4000 \text{ MPa}$,
 175 $Q_{WC} = 3000 \text{ MPa}$ and $b_{WC} = 10$ are given for a uniaxial compression loading of the WC.

176 2.2.2 Drucker Prager criterion for the carbide WC phase

177 Tkalich *et al.* [24] used the Drucker Prager model [39] for the WC phase initially developed for soil
 178 mechanics. Thanks to its dependence on pressure, this model can reproduce the difference in
 179 behaviour between tension and compression. This difference is highlighted by the experiments carried
 180 out by Doi *et al.* [40] where tensile tests not exceed 0.7% of deformation and a maximal tensile stress
 181 of 210 MPa while compression tests reach the maximum of 4% of deformation and a maximal
 182 compressive stress of 335 MPa for a WC-20wt.% Co with a WC grain size of 2.1 μm . In the present
 183 work, this criterion, already implemented in ABAQUS code, is also adopted for the carbide phase to
 184 compare it with the von Mises criterion presented above.

185 The Drucker Prager criterion is defined as follows:

$$186 \quad f_{WC}(\boldsymbol{\sigma}, p) = \sigma_{eq} - (R_{WC} + Y_{WC}(p)) \quad (5)$$

187 where the equivalent stress is $\sigma_{eq} = \frac{J_2(\boldsymbol{\sigma}) + I_1(\boldsymbol{\sigma}) \tan(\phi_{WC})/3}{1 - \tan(\phi_{WC})/3}$ with $I_1(\boldsymbol{\sigma}) = \text{trace}(\boldsymbol{\sigma})$ is the stress tensor
 188 trace and ϕ_{WC} , the friction angle that is set to 45°, implying that the yield stress in uniaxial tension is
 189 half as large as in compression [24]. In Equation (5), the term $R_{WC} + Y_{WC}(p)$ is given by Equation (4).
 190 The accumulated plastic strain p which is defined by :

$$191 \quad p = \int_0^t \frac{\boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}^p}{\sigma_{eq}} dt \quad (6)$$

192 the plastic strain rate $\dot{\boldsymbol{\epsilon}}^p$ is calculated from the following non-associated flow rule :

$$193 \quad \dot{\boldsymbol{\epsilon}}^p = \dot{\lambda} \frac{\partial g_{WC}}{\partial \boldsymbol{\sigma}} \quad (7)$$

194 with $\dot{\lambda}$, the plastic multiplier and g_{WC} flow potential defined as :

$$195 \quad g_{WC}(\boldsymbol{\sigma}) = J_2(\boldsymbol{\sigma}) + \frac{1}{3} I_1(\boldsymbol{\sigma}) \tan(\psi_{WC}) \quad (8)$$

196 where ψ_{WC} is the dilatation angle. In this paper an associate flow rule is considered, i.e. $\psi_{WC} = \phi_{WC}$.

197 In the Drucker Prager model, the hardening parameters and yield stress must be determined from a
198 stress-plastic strain curve obtained in monotonic uniaxial compression test. It is interesting to note that
199 under this loading condition, the yield function is identical for both elastoplastic models:

$$200 \quad f(\boldsymbol{\sigma}, p) = |-\sigma_{comp}| - R - Y(p) \quad (9)$$

201 as well as the cumulated plastic strain p computed as follows (see the proof in **Appendix A**):

$$202 \quad p = \int_0^t |-\dot{\varepsilon}_{comp}^p| dt \quad (10)$$

203 where $\sigma_{comp} > 0$ and the $\dot{\varepsilon}_{comp}^p > 0$ are the normal stress and plastic strain rate in the direction of the
204 compression.

205 In the following of this study, the von Mises criterion for both phases will be used in the development
206 of this microstructural model. The results of the model will be compared to those calculated from the
207 von Mises and Drucker-Prager criteria applied respectively to the Co and WC behaviours in
208 Subsection 5.4.

209
210

2.3 Interfaces

211 In the composite, two types of interfaces can be observed: WC/Co and WC/WC. In simulations
212 dealing with the behaviour of composites at the microstructure scale, the WC/Co interfaces are
213 represented geometrically. These interfaces are considered as a perfect contact because of the good
214 adhesion between these two phases [24, 25]. This good adhesion can be justified during sintering by a
215 low interfacial energy which leads to an excellent wetting of the cobalt on the WC grains [41].
216 Regarding WC/WC interfaces, Csanadi *et al.* [42] concluded from micro-bending tests that their
217 bending strength is generally lower than that of the WC grains. Sometimes, these interfaces are
218 represented geometrically in some models but there are considered generally as perfect [24–26]. Their
219 elasto-plastic models, like those presented in Subsection 2.2, are dedicated to polycrystalline materials.
220 Therefore, the influences of grain boundaries are implicitly included in the parameters of these
221 models. The WC/WC interfaces that will be represented in the present work are also considered as
222 perfect.

223 3. Creation of the microstructure

224 Simulations are based on a geometrical representation of the microstructure. However, various
225 complex geometries of the WC-Co microstructure are represented in the literature. In several
226 investigations lead by Sadowski *et al.* [22, 32], the composite consists of polygonal WC grains
227 surrounded by a thin layer of cobalt. Faksa *et al.* [26] have also adopted this description in part of their
228 work, which is named "Co-matrix model". Nevertheless, in most representations of the WC-Co
229 microstructure, the WC grains are in contact to form a WC skeleton with WC/WC interfaces that are

230 excluded in the “Co-matrix model”. The presence of such skeleton was first formulated by Dawihl and
231 Hinnüber [43], observing that the samples maintained their shape after the cobalt had been attacked by
232 boiling HCl. The existence of this skeleton, if any, is conditioned by the cobalt content. However, the
233 percentage of cobalt above which the skeleton is no longer obtained is not well defined. For instance,
234 Exner [3] fixed that limit to 30 wt.%Co while it is about of 11 wt.%Co for Dawihl and Hinnüber [43].
235 In 2D observations, the cobalt phase seems to be isolated in small areas, especially when the weight
236 percentage of Co is low. Faksa et al. [26] also adopted this description which is named "WC-matrix
237 model". According to the results of their research, this microstructural description is more appropriate
238 to represent the elastoplastic behaviour of the composite. However, the hypothesis of an isolated Co
239 phase is no longer necessarily true in the case where the weight percentage of Co increases. Some
240 authors have shown continuous Co skeletons on several WC-Co grades in 3D space [44]. In addition,
241 the distribution of cobalt in the WC-Co composite is not uniform. List et al. [45] observed, on the rake
242 face of an uncoated carbide insert (geometry type K4, Sandvik) H13A grade (K20, 6%Co), based on a
243 SEM images, some areas rich in cobalt and others in carbide grains.

244 Due to the complexity of the WC-Co microstructure, most microstructural simulations in the literature
245 generally use a 2D geometric representation of the microstructure generated from microscopic images.
246 For example, Zhu et al. [31] have structured this process in their research in six steps: noise reduction,
247 image binarization, WC grain segmentation, WC grain boundary definition, WC grain boundary
248 vectorization and meshing. Recently, Jiménez-Piqué et al. [44] have reconstructed a 3D microstructure
249 from a sequence of images obtained by FIB (Focused Ion Beam Tomography). However, these studies
250 are limited by the number of micrographs and obtaining them is a long process. Alternatives are also
251 proposed in the literature where an idealized WC-Co microstructure is rapidly generated from an
252 algorithm for a given wt.% of Co. For example Park et al. [38] proposed an algorithm to build a 2D
253 WC-Co microstructure. In their work, a single WC grain is defined by a quadrangle controlled by four
254 parameters: a centroid, a major axis, a minor axis and the orientation angle measured between a major
255 axis and a horizontal reference line. The values of these parameters are defined from statistical
256 distributions determined on real microstructures. The quadrangles are randomly distributed to generate
257 a WC skeleton. The voids between the WC grains are filled by the Co phase. Kayser et al. [46] used
258 truncated prisms for the WC grains and generated a 2D microstructure which is extruded in the third
259 direction.

260 In the present paper, 2D square microstructures have been created in Matlab using the algorithm
261 proposed by Tkalich et al. [25]. The microstructures are generated from the Voronoi cell pattern. Then
262 each cell is divided into two parts by a line. Each part of the cell contains either the WC phase or the
263 Co binder. The temporary crossing point of this line is randomly placed on an edge of the cell. The
264 line makes a randomly imposed angle α with the horizontal in the interval $[0; \pi]$. Then, the shortest

265 distance between the farthest cell vertex and the line is iteratively calculated such that the predefined
266 surface fraction of the binder phase is reached with an accuracy of more than 98%.

267 Finally, RVE is extruded to over 1/10 of its lateral length in the third direction as in [47] to perform a
268 3D computation (see Figure 4). This algorithm makes it possible to rapidly generate a large number of
269 idealized microstructures (or RVE) with different Co contents to analyse its effect on the elasto-plastic
270 behaviour of the composite. Nevertheless, it is necessary to define a minimum number of cells to
271 generate RVEs that will allow to represent the elasto-plastic behaviour of the WC/Co with a good
272 accurate. This cell number is studied in following section.

273 **4. RVE determination**

274 In the literature, the RVE is often defined by the number of WC grains, although their behaviour is
275 that of a polycrystalline WC in the numerical simulations. The number of WC grains and Voronoi
276 cells are identical and controls indirectly the distribution of the cobalt phase. Thus, a large number of
277 WC grains leads to a more homogeneous distribution and smaller islets of cobalt in the microstructure,
278 as shown in Figure 5. In this work, 8 groups of microstructures comprising 5, 50, 100, 150, 200,
279 250, 275, 300 WC grains are studied for composites of WC-6wt.%Co and WC-20wt.%Co. These two
280 compositions have been chosen to determine an RVE covering a wide range of cobalt content used in
281 cutting tools. For each group, 4 different microstructures have been generated. For all microstructures,
282 simulations have been performed using the finite element method implemented in the ABAQUS
283 Software [37]. Each RVE is subject to kinematic boundary conditions showed in Figure 6 to simulate
284 a uniaxial compression test. This test allows the comparison between the results of the simulation and
285 the experimental data in the literature. As shown in Figure 6, at the left, on the bottom and at the back
286 of the sides of the microstructure, displacements are fixed in the x , y and z directions, respectively. On
287 the upper side (at the left side), a negative displacement $-u_y$ ($-u_x$) is imposed to performed uniaxial
288 compression in the y (and x) directions. The remaining sides, a relationship between nodes could be
289 applied to impose straight sides. However, Sadowski *et al.* [22] compared this solution with that of
290 free sides and obtained the same results. In the present study, these sides are free. The element type
291 used is a linear prismatic element C3D6 with 6 nodes. A suitable mesh size has been selected from
292 convergence studies for each RVE. For illustrative purposes, Figure 7 shows the normalized Young's
293 modulus and dissipated plastic energy computed with different mesh sizes on RVE of 275 grains. The
294 tested element sizes are 0.042, 0.031, 0.012, 0.007 and 0.005 of the RVE size corresponding to 3595,
295 4868, 35280, 65631 and 101418 elements. In the following of this study, the third mesh size has been
296 selected.

297 The criteria to determine the RVE are partly inspired by those proposed by Chen *et al.* [23]. The first
298 criterion is the ratio E_x/E_y where E_x and E_y are the apparent Young's moduli of each microstructure
299 obtained from simulations of uniaxial compression in the x and y directions, respectively. If this

300 criterion is close to one, then the microstructures are considered isotropic. In Figure 8, the averages of
301 ratio E_x/E_y for each group of microstructures are plotted as a function of the number of grains. For
302 composites containing 6 wt.%Co, this ratio is approximately equal to 1 with an error of less than 1%
303 regardless the number of grains, whereas for its counterpart containing 20wt.%Co, this error is reached
304 from 100 grains upwards. Moreover, for all groups of microstructures larger than 100 grains, as shown
305 in Figure 8, the dispersion of this criterion in each group is low since its standard deviation is less than
306 0.01. A low standard deviation means that the apparent properties of the RVE are not affected by
307 different microstructures containing the same number of grains. For microstructures with less than
308 100 grains, the standard deviation is higher because the distribution of the cobalt phase is very
309 heterogeneous.

310 The second criterion is defined as the ratio E_i/E_{300} , where E_i and E_{300} are the mean Young's moduli
311 of the microstructure groups containing i and 300 grains, respectively. Microstructures composed of
312 300 grains are taken as a reference since they have the largest number of grains in this study.
313 Moreover, it is likely that their apparent mean Young's modulus already converges to the effective
314 Young's modulus of the composite as observed by Chen *et al.* in [23]. The E_{300} values for the WC-
315 6wt.%Co and WC-20wt.%Co composites are 623 and 480 GPa, respectively. Figure 9 shows a
316 variation of the ratio E_i/E_{300} and its standard deviation as a function of the number of grains. As for
317 the previous criterion, from 100 grains upwards, all ratios E_i/E_{300} are close to 1 with an error of less
318 than 1% and a standard deviation of less than 0.01. In other words, the ratio converges quickly, and the
319 apparent Young's modulus of the microstructures is close to the values of E_{300} . The same trends are
320 also observed for Poisson's ratio and thermal expansion. However, as mentioned by Chen *et al.* in
321 reference [23], the RVE defined with the elastic phases cannot be sufficient to perform a plastic study
322 of the composite due to the development of the overall non-linearity of the material. It is therefore
323 necessary to continue this study by selecting a criterion for the determination of the RVE taking into
324 account the plastic behaviour of each phase.

325 The third criterion is the P/U ratio where P and U are respectively the average plastic energy
326 dissipated and the external work, for a total deformation of 2% obtained by simulating a uniaxial
327 compression test. Figure 10 shows the mean value of the P/U ratio and its standard deviation as a
328 function of number of grains for the two cobalt grades. The P/U ratio begins to converge towards the
329 value of about 0.46 and 0.38 from 200 grains for microstructures containing 6 and 20 wt.% of cobalt,
330 respectively, with standard deviations less than 0.01. As suspected, the number of grains where this
331 criterion converges is greater than that observed in the elasticity studies.

332 Note that a final criterion often used in the literature to determine an RVE can also be applied. This is
333 the Hill's criterion, which is independent of the mechanical behaviour under consideration. According
334 to Chen *et al.* [23], this criterion can be written as follows :

335
$$\psi = \max\left(\frac{\langle\sigma\rangle:\langle\varepsilon\rangle}{\langle\sigma:\varepsilon\rangle}, \frac{\langle\sigma:\varepsilon\rangle}{\langle\sigma\rangle:\langle\varepsilon\rangle}\right) \quad (11)$$

336 If this criterion tends towards 1, then the RVE is correctly defined. Figure 11 shows the mean value of
337 ψ and its standard deviation as a function of the number of grains. ψ is equal to 1 for the composite
338 WC-6wt.%Co while its counterpart with WC-20wt.%Co decreases to converge towards 1.16 from 250
339 grains. For microstructures larger than 250 grains, the standard deviations of ψ for both grades are less
340 than 0.01.

341 According to the different criteria defined above, an RVE with a number of grain greater than 250 can
342 be selected with confidence. A RVE with 275 WC grains is selected in the following. This number is
343 comparable to the one found by Chen *et al.* Sadowski *et al.* [22] for a RVE with a size of 40x40 μm
344 and an average tungsten carbide grain size of 2.35 μm (i.e. 290 WC grains for a cobalt-free
345 composite).

346 **5. Results and discussion**

347 The RVE being defined, the numerical model is tested to validate its ability to reproduce the elastic
348 and elasto-plastic experimental behaviours of the composite.

349 **5.1 Elastic behaviour validation of the model**

350 The validation of the elastic behaviour of the model consists in predicting the Young's moduli of
351 composites containing 6, 10, 12 and 20 wt.% Co (0.9, 0.83, 0.8 and 0.675 WC volume fraction
352 respectively) and comparing them with experimental data obtained in the literature [48–51], see Figure
353 12.

354 For each composite, four quasi-realistic microstructures have been generated. The calculated
355 maximum deviation is less than 0.6%. Consequently, the error bar corresponding to the dispersion of
356 the results of the realizations is not visible on Figure 12. A good agreement between the calculated and
357 measured Young's moduli is obtained, in particular with the data provided by Schwartzkopf and
358 Kieffer [48]. The numerical results are included in the scatter of the experimental data set which is of
359 the order of about 50 GPa for the same cobalt content. The increase in Young's modulus as a function
360 of WC volume fraction is also well reproduced. This test was often used in the literature by Jaensson
361 and Sundström [19], and Tkalich *et al.* [24] to evaluate the robustness of the model.

362 **5.2 Elastoplastic behaviour validation of the model at room temperature**

363 The second validation is the reproduction of the stress-strain curve measured by Tepperneegg *et al.* [30]
364 up to a total strain of 2% for a WC-6wt.%Co composite in uniaxial compression at room temperature,
365 see Figure 13. In Figure 13, the simulated stress-strain curves with the hardening parameters taken
366 from the work of Tkalich *et al.* [24] ($Q_{WC} = 3000 \text{ MPa}$ and $b_{WC} = 10$) reproduce the experimental

367 data up to 0.5% strain. Beyond this deformation, the hardening of the composite calculated by the
368 model is lower than that observed on the experimental curve. The stress is underestimated up to 33%
369 of the measured value for a 2% deformation. The hardening parameters used do not seem adequate to
370 reproduce the experimental data. However, the stress-strain curves of the composite depend on the
371 WC grain size [40]. The experimental curves measured by Teppernegg *et al.*, used as a reference for
372 this study, were measured on composites with a grain size of about $1\mu m$. Therefore, the hardening
373 parameters Q_{WC} and b_{WC} of the carbide phase must be redefined so that the simulated curve
374 corresponds to that measured on the composite knowing that the elastoplastic behaviour of cobalt is
375 already defined. Although the WC grain size effect on the composite is beyond the scope of the
376 present paper, this one would be considered by Hall-Petch type relationships in the elasto-plastic
377 models [52, 53]. Indeed, this size cannot be considered using the geometry of the microstructure
378 generated in Section 3 because the models are based on the continuum mechanics theory insensitive to
379 the absolute size, [21].

380 The first parameter Q_{WC} represents the difference between the maximal compressive stress that the
381 WC phase can achieve and its compressive yield stress R_{WC} . If Q_{WC} is zero, the material is perfectly
382 plastic. The second parameter b_{WC} controls the growth rate of the stress in the elastoplastic regime of
383 the WC. These parameters, despite of the presence of the cobalt, seems to have the same influence on
384 the composite behaviour. Indeed, when only Q_{WC} increase up to 6000 MPa with $b_{WC} = 10$, the stress
385 of the composite rises from 3925 MPa to 4200 MPa for strain of 2%, see Figure 13. If b_{WC} is
386 multiplied by 50, the stress increases rapidly. For a strain of 1%, the slope of the curve for $b_{WC} = 500$
387 is equal to 2520 MPa/% versus 570 MPa/% for $b_{WC} = 10$. The combination $Q_{WC} = 3000 MPa$ and
388 $b_{WC} = 500$ has been found by trial and error to be in good agreement with the experimental
389 counterpart and will be use in the following of this paper. By comparison with the values of Q_{WC} and
390 b_{WC} proposed by Tkalich *et al.* [24, 25], only the last parameter changes.

391 In conclusion of this section, the mechanical behaviour of the composite can be represented from these
392 phases and especially from the carbide phase which is fully defined at room temperature. The stress-
393 strain curves of Co and WC are the lower and upper limits, respectively, of the composite behaviour as
394 shown in Figure 14. If both phases are considered elastic, this assumption is valid for deformations of
395 less than 0.4% as shown in the WCECoE curve (WC elastic; Co elastic). In the case where only cobalt
396 has an elasto-plastic behaviour (see the WCECoP (WC elastic; Co plastic) curve in Figure 14) as in
397 the studies of several authors [19, 21, 32, 40], this model is valid up to deformations of 0.6%. Beyond
398 this deformation, the plasticity of the cobalt in the model is no longer sufficient to reproduce the
399 experimental curve of the composite. This observation shared by Faksa *et al.* [26] led the authors to
400 introduce the plasticity of the carbide. Poech *et al.* [21], indicated that it is necessary to take into
401 account the plasticity and/or damage processes in the carbide phase after the initial plasticity of the
402 composite. However, according to the results of Tkalich *et al.* [24], plasticity is activated in the WC

403 phase well after that of cobalt in the composite due to the lower yield stress of cobalt. This tendency is
404 also observed in the present model because the curve considering the plasticity of the two phases
405 (WC-CoP) merges with the WCECoP curve before a deformation of 0.6%. Finally, the WC-CoP
406 deformation curve reproduces the response of the WC-Co composite under uniaxial compressive
407 loading up to 2% deformation.

408 **5.3 Simulation of the composite at different temperatures**

409 So far, simulations previously carried out have been limited to room temperature. As presented in the
410 introduction, the composite WC-Co used in cutting tools are subjected to different temperatures during
411 machining. Therefore, the effect of temperature must be taken into account in this modelling. The
412 Young's modulus and the thermal expansion of Co and WC are already dependent on temperature as
413 well as the elastoplastic behaviour of the Cobalt phase, see Section 2. In order to complete the present
414 modelling, it is necessary to have compressive stress-strain curves of the WC for different
415 temperatures **which are scarce in the literature**. To overcome this obstacle, a strategy similar to that
416 proposed by Faksa et al. [26] was adopted by reconstructing the WC behaviour from Co and a
417 composite WC-6wt.%Co. For the composite, the compressive stress-strain curves were measured by
418 Teppernegg et al. [30] up to 2% strain at temperatures of 25, 200, 400, 600, 800 and 900°C, see Figure
419 16.

420 In order to take temperature into account in the plastic regime of the carbide phase, the following
421 modification of the yield criterion was introduced :

$$422 \quad f_{WC}(\boldsymbol{\sigma}, p, T) = \sigma_{eq} - R_{WC}(T) - \alpha_2(T)Y_{WC}(p) \quad (12)$$

423 with $R_{wc}(T)$ defined as following :

$$424 \quad R_{wc}(T) = \alpha_1(T)R_{wc}(T = 25^\circ) \quad (13)$$

425 $\alpha_1(T)$ and $\alpha_2(T)$ control the temperature dependence of the yield stress $R_{wc}(T)$ and the isotropic
426 hardening of the WC material, respectively. Note that for $T = 25^\circ\text{C}$, $\alpha_1 = \alpha_2 = 1$. This modification
427 is valid for both von Mises and Drucker Prager criteria since their compressive stress-strain curves are
428 equivalent **changes**. The parameters α_1 and α_2 will implicitly include the observed modifications in
429 the behaviour of WC-Co with increasing temperature. Mari [15], this change occurs from 527°C and is
430 explained by an increase in toughness induced by the softening of cobalt under limited plastic
431 deformation. The sliding of WC grain boundaries is one of the mechanisms involving this softening as
432 reported by several authors [15, 54]. Above 827 °C, the behaviour of the composite is entirely plastic.

433 For the reconstruction of the elasto-plastic behaviour of the WC, the temperature-dependent evolution
434 of one of the parameters will be imposed while the other will be defined from the compressive stress-
435 strain curves of the composite for different temperatures.

436 $\alpha_1(T)$ has been calculated assuming that the evolution of the ratio $\sigma_{wc-}(T)/\sigma_{wc-Co}(T = 25^\circ C)$ of
437 the composite is the same as that of the WC material. $\sigma_{wc-Co}(T)$ and $\sigma_{wc-Co}(T = 25^\circ C)$ are the
438 stresses of the composite measured at a given temperature and at room temperature, respectively, for a
439 plastic deformation of 0.2%. This assumption may be rough, but it ensures that the yield stress of WC
440 is always higher than that of the composite. Indeed, as shown in Figure 14, the behaviour of the
441 composite is between that of carbide and cobalt. It allows the cobalt to deform plastically over a wide
442 range of strains before the carbide deformations occur in the composite. $\alpha_2(T)$ have been determined
443 by performing several simulations to reach, by trial and error, a good agreement with the experimental
444 stress-strain curves of the composite, see Figure 16. The values of $\alpha_1(T)$ and $\alpha_2(T)$, shown in Figure
445 15, decrease gradually as the temperature increases. Nevertheless, their respective evolutions are
446 independent although $\alpha_1(T)$ and $\alpha_2(T)$ are close for 200, 400, 800°C. In other words, the evolution of
447 the yield stress as a function of temperature is not dependent on that of the hardening.

448 The plastic stress-strain curves of the WC in compression can be plotted for different temperatures as
449 shown in Figure 17 and compared with the results obtained by Faksa et al. [26]. Let us recall that these
450 authors determined the behaviour of the WC, with a similar strategy, more precisely, from those of the
451 composite WC-6wt.%Co and a cobalt alloy. The orders of magnitude of the stresses are almost
452 similar, except for the shape of the curves and the yield stress. The shape of the curves in this case is
453 imposed by the relation (4), while those of Faksa et al. are obtained directly from the simulation
454 results. The yield stresses of WC obtained by these authors overestimates by 1 GPa those of this paper
455 for temperatures of 25°C, 200°C, 400°C. However, they are almost identical for temperatures above
456 600°C. It can be noted that the determination of the yield stress of WC is not obvious because
457 according to Csanádi et al. [55], the tolerance in its measurement can reach 1 GPa.

458 As the parameters $\alpha_1(T)$ and $\alpha_2(T)$ are determined from the data of the composite WC-6 wt.%Co, the
459 model is applied to compression tests of a composite WC-10.5wt.%Co measured by Tepperneegg et al.
460 [30] for different temperatures, see Figure 18. All model parameter values are summarised in Table 1.
461 For temperatures above 600°C, the model overestimates the experimental curves for a strain of 0.25%
462 at T=900°C. On the other hand, for temperatures less than or equal to 600°C, the simulations
463 underestimate the experimental data with a maximum error of 30 % for a strain of 0.3% at T=600°C.
464 Note that the difference between the calculated and measured curves reduces as the temperature
465 decreases. The modelling correctly predict the measured stress-strain curves, especially for strains
466 greater than 1% (except for the one obtained at 900°C). After 800°C, the elasto-plastic laws used in
467 the present modelling seem less appropriate as the material becomes more sensitive to strain rate
468 (Smith and Wood 1968). Tepperneegg's et al. (Tepperneegg et al. 2016) obtained experimental data with
469 an imposed strain rate of $5 \cdot 10^{-3} s^{-1}$ corresponding to that encountered in creep tests (Sakuma
470 and Hondo 1992). For high temperatures, visco-plastic models would be more suitable to reproduce
471 the behaviour of carbide and cobalt phases.

5.4 Comparison between the models using von Mises and Drucker Prager criteria for

WC

So far, simulations presented above have been performed with the von Mises criterion applied to the carbide phase. The hardening parameters $Q_{WC} = 3000 \text{ MPa}$ and $b_{WC} = 500$ as well as the parameters $\alpha_1(T)$ and $\alpha_2(T)$ found previously have been also applied for the Drucker Prager criterion. Figures 19 and 20 show a comparison between these two criteria on the stress-strain curves computed at different temperatures for the carbide grades WC-6wt.%Co and WC-10.5wt.%Co, respectively. The curves computed with both criteria for the WC-6wt.%Co composite are almost identical, when the behaviour of the WC phase is determined with the von Mises criterion, the average stress tensor, shown by the relation (14), is close to a state of uniaxial compressive stress.

$$\boldsymbol{\sigma} = \begin{pmatrix} 241 & -4.4 & 0.9 \\ -4.4 & -6106 & -1.3 \\ 0.9 & -1.3 & 278 \end{pmatrix} \text{ MPa} \quad (14)$$

This tensor has been computed at room temperature and for a strain of 2%. The same case for the stress tensor was computed with the Drucker Prager criterion, see relation (15).

$$\boldsymbol{\sigma} = \begin{pmatrix} 150 & -5.9 & 0.7 \\ -5.9 & -5946 & -0.9 \\ 0.7 & -0.9 & 170 \end{pmatrix} \text{ MPa} \quad (15)$$

As mentioned in Section 2.2.2 and **Appendix A**, for this mechanical loading, the two models are equivalent explaining the curves superpositions of Figure 19.

However, the stress states calculated at each integration point are locally different due to the complex shape of the WC phase and can be represented by points in a diagram $p - J2$ in order to analyse their dispersion. This type of diagram also used by Tkalich *et al.* [25] is plotted for both criteria in Figures 21(a) and (b) at room temperature for a total strain of 2%. Most of these points are concentrated in the vicinity of the bold red line which represents the load path for a uniaxial compression. The green and blue lines symbolize the initial and maximum yield stresses, respectively. In Figure 21(b), these last two lines are tilted in the case of the Drucker Prager model because of its dependence on pressure. For this model, the diagram clearly shows the difference between the compressive and tensile yield stress with a shorter load path for the tensile depicted by the blue line. Another difference between these two criteria is that certain stress states may exist in one of these two models and not in the other. For example, in Drucker Prager's model for high pressures, some points are above the maximum yield stress of the Mises model, see Figure 21(a). The opposite can be observed for low pressures, where some points calculated with the von Mises criterion are above the maximum yield stress of the Drucker Prager criterion. However, this concerns only a few points and has no impact on the stress-strain curves of this composite in compression as shown in Figure 19.

503 As the cobalt content increases, the shape of the WC phase becomes more complex and involves more
504 varied stress states in the microstructure. In the case of the composite WC-10.5wt.%Co, the dispersion
505 of the points is greater with an increase in the number of areas in the microstructure with low plasticity
506 in the WC as shown Figures 21(c) and d. For the Drucker Prager model, in Figure 21(d) a shift of most
507 of the points from the compression path towards low pressures in the diagram $p - J_2$, is also observed.
508 These data have been calculated for both criteria at room temperature for a total strain of 2%. In this
509 case, the average stress state gets away from a uniaxial compressive mechanical load and therefore
510 these models are no longer equivalent. That is why there is a slight difference between the curves in
511 Figure 20 calculated according to these two criteria. The discussions and comments written in the
512 previous section between the experimental data and the results of the von Mises model can be applied
513 to the Drucker Prager model.

514 For future simulations at the microstructural scale, the Drucker Prager criterion is better suited to
515 represent the behaviour of the WC phase because it can simulate the difference between the tension
516 and compression behaviours observed in the composite.

517 **6. Conclusions and Perspectives**

518 In this paper, a microstructure scale modelling has been proposed to simulate the elastoplastic
519 behaviour of the WC-Co composite with different contents of cobalt and various temperatures from 25
520 to 900 °C.

521 The elastoplastic behaviour of each phase has been identified from the literature. The cobalt has been
522 modelled with the von Mises criterion for its plastic behaviour. This criterion and the Drucker Prager
523 one have been used in the first instance for the tungsten carbide phase at room temperature. Although
524 its behaviour is often considered elastic, it has been extended to the field of plasticity to simulate the
525 compression of the composite for strains greater than 0.6%. The properties at the WC-WC and WC-Co
526 interfaces as well as the WC grain size effect have not been considered. Thereafter, realistic
527 microstructures have been generated by an algorithm inspired from the work of Tkalich et al. [25] to
528 control the grain number of WC and the cobalt content.

529 Then, a study has been led to determine the WC grain minimum number in a representative volume
530 element to reproduce the macroscopic behaviour of the composite in compression. The convergence of
531 the criteria as the isotropy of the elastic behaviour, the Young's modulus, the ratio between the
532 dissipated plastic energy and the external work and the Hill's criterion have been achieved for
533 microstructures which the number of WC grain is larger than 250.

534 In the following of this study, the hardening parameter of plastic behaviour models for the carbide
535 phase have been determined $Q_{WC} = 3000 \text{ MPa}$ and $b_{WC} = 500$ from the uniaxial compression tests
536 performed on a grade WC-6wt.%Co at room temperature. Then, the yield criterion has been extended

537 to different temperatures by the introduction of two functions $\alpha_1(T)$ and $\alpha_2(T)$. These two parameters
538 represent the dependence of the yield stress and hardening on temperature, respectively. These
539 functions have been determined with a microstructure of 275 grains from the elastoplastic behaviour
540 of the cobalt and composite WC-6wt.%Co for a temperature range of [20-900°C] with the von Mises
541 model.

542 Simulations have been performed to predict the stress-strain curves in compression of the composite
543 WC-10.5wt.%Co compared with experimental data taken from the work of Tepperneegg *et al.* [30]. A
544 good agreement was observed for all temperatures for a strain larger than 1% excepted for 900°C.
545 Before this strain, the model overestimates and underestimates the experimental curves for
546 temperatures larger and lower than 600°C, respectively.

547 A comparison between the von Mises and Drucker Prager criteria applied to the carbide phase have
548 been also discussed. Both models lead to equivalent results in uniaxial compression. Nevertheless, the
549 local stress states between these approaches become different when the cobalt content increases.
550 However, it is recommended to use Drucker Prager criterion because it can reproduce the difference
551 between yield stress in traction and compression observed in the composite.

552 The model presented in this work assumes that the decrease in the stress rate for large deformations is
553 only due to plastic deformations. Possible extensions and improvements can be proposed in
554 forthcoming work, such as considering the damage and the visco-plastic behaviour of the composite
555 phases. In addition, the used plastic models neglect the WC and Co grain size and their orientation. It
556 would be interesting to use the crystal plasticity for both phases for a more accurate description of the
557 composite behaviour.

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566 **Appendix A. Proof of the equivalence of the von Mises and Drucker**
567 **Prager elasto-plastic models under a compression loading**

568 The following appendix shows that the plastic stress-strain curves of the uniaxial compression test
569 obtained in the compression axis are equivalent for the Mises and Drucker Prager models if $\phi_{WC} =$
570 $\psi_{WC} = 45^\circ$. Only the quantities useful for this proof are defined. For more information on undefined
571 quantities, please refer to Section 2. The *MS* and *DP* indices attached to the quantities refer to the von
572 Mises and Drucker Prager models.

573 In the uniaxial compressive test, Cauchy stress tensor is written as follow :

$$574 \quad \boldsymbol{\sigma} = \begin{bmatrix} -\sigma_{com} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (\text{A.1})$$

575 with $\sigma_{com} > 0$, the magnitude of the stress in the direction of compression.

576 The yield surface for both models is

$$577 \quad f_{WC}(\boldsymbol{\sigma}, p) = \sigma_{eq} - (R_{WC} + Y_{WC}(p)) \quad (\text{A.2})$$

578 In the von Mises model, the equivalent stress is $\sigma_{eqMS} = J_2(\boldsymbol{\sigma})$. For the stress state of (A.1), $\sigma_{eqMS} =$
579 σ_{com} . In the Drucker Prager model, the equivalent stress is $\sigma_{eqDP} = \frac{J_2(\boldsymbol{\sigma}) + I_1(\boldsymbol{\sigma}) \tan(\phi_{WC})/3}{1 - \tan(\phi_{WC})/3}$ with $\phi_{WC} =$
580 45° . For the stress state of (A.1), the equivalent stress is also the one computed with the Mises model,
581 i.e. $\sigma_{eqDP} = \sigma_{com}$.

582 In relation (A.2), the accumulated plastic strain p , for the von Mises model is defined as follow :

$$583 \quad p_{MS} = \int_0^t \dot{\epsilon}_{eqMS} dt = \int_0^t \sqrt{\frac{2}{3} \dot{\boldsymbol{\epsilon}}_{MS}^P : \dot{\boldsymbol{\epsilon}}_{MS}^P} dt \quad (\text{A.3})$$

584 with plastic strain rate equivalent $\dot{\epsilon}_{eq}$ which is computed from the plastic strain rate tensor

585 $\dot{\boldsymbol{\epsilon}}_{MS}^P$ computed from the associate flow rule :

$$586 \quad \dot{\boldsymbol{\epsilon}}_{MS}^P = \dot{\lambda} \frac{\partial f_i}{\partial \boldsymbol{\sigma}} \quad (\text{A.4})$$

587 In the case of the stress state given in (A.1), the plastic strain is :

$$588 \quad \dot{\boldsymbol{\epsilon}}_{MS}^P = -\dot{\epsilon}_{com} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix} \quad (\text{A.5})$$

589 with $\dot{\epsilon}_{com} > 0$ the magnitude of the strain rate plastic deformation in the compressive direction.

590 Therefore, the plastic strain rate equivalent is $\dot{\epsilon}_{eqMS} = \dot{\epsilon}_{com} > 0$.

591 For the Drucker Prager model, the accumulated plastic strain is defined as :

592
$$p_{DP} = \int_0^t \dot{\epsilon}_{eqDP} dt = \int_0^t \frac{\sigma: \dot{\epsilon}_{DP}^P}{\sigma_{eqDP}} dt \quad (A.6)$$

593 With equivalent plastic strain rate $\dot{\epsilon}_{eqDP}$ which is computed from the plastic strain rate tensor $\dot{\epsilon}_{DP}^P$
594 obtained from the flow rule :

595
$$\dot{\epsilon}_{DP}^P = \lambda \frac{\partial g_{WC}}{\partial \sigma} \quad (A.7)$$

596 The flow potential for $\psi_{WC} = 45^\circ$ is :

597
$$g_{WC}(\sigma) = J_2(\sigma) + \frac{1}{3} I_1(\sigma) \tan(\psi_{WC}) \quad (A.8)$$

598 In the case of the stress state given in (A.1), the plastic strain is :

599
$$\dot{\epsilon}_{DP}^P = -\dot{\epsilon}_{com} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{15}{12} & 0 \\ 0 & 0 & -\frac{15}{12} \end{pmatrix} \quad (A.9)$$

600 Therefore, the equivalent plastic strain rate is $\dot{\epsilon}_{eqDP} = \dot{\epsilon}_{com}$ which is identical to the one computed
601 with the von Mises model.

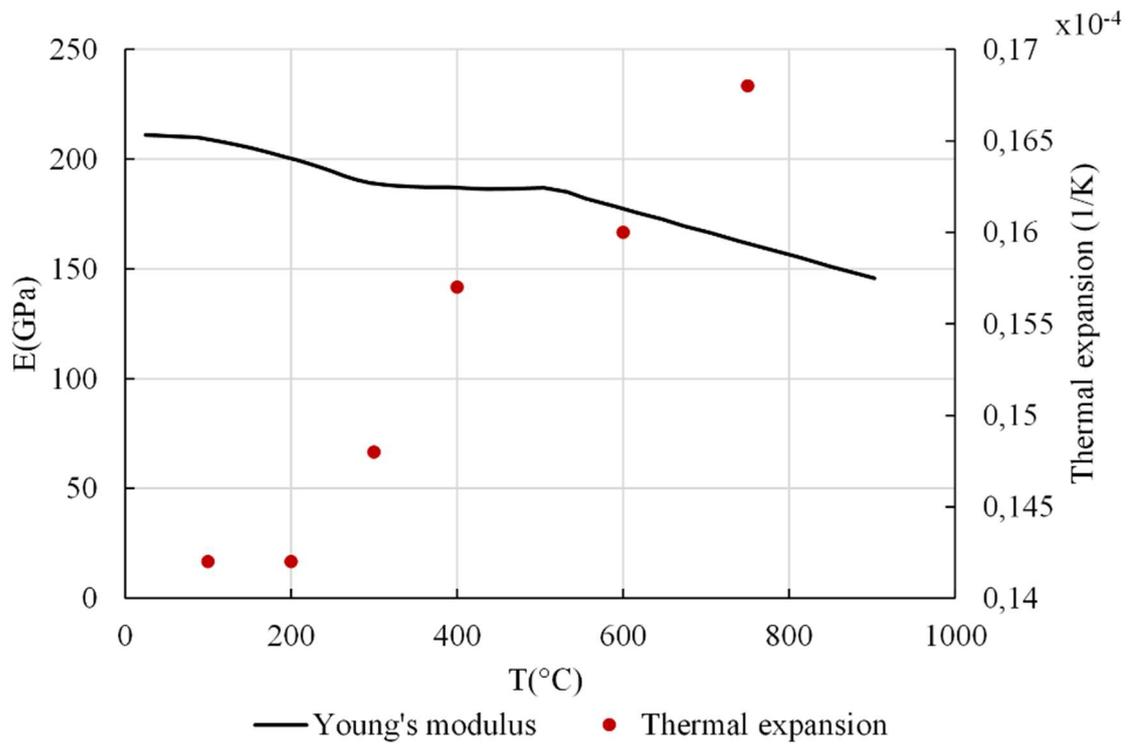
602 To conclude, for both models, the accumulated plastic strain is

603
$$p = \int_0^t \dot{\epsilon}_{com} dt = \epsilon_{com} \quad (A.10)$$

604 as well as the yield surfaces are the same. Consequently, the curves $(\sigma_{comp}, \epsilon_{com})$ plotted for these
605 models are equivalent.

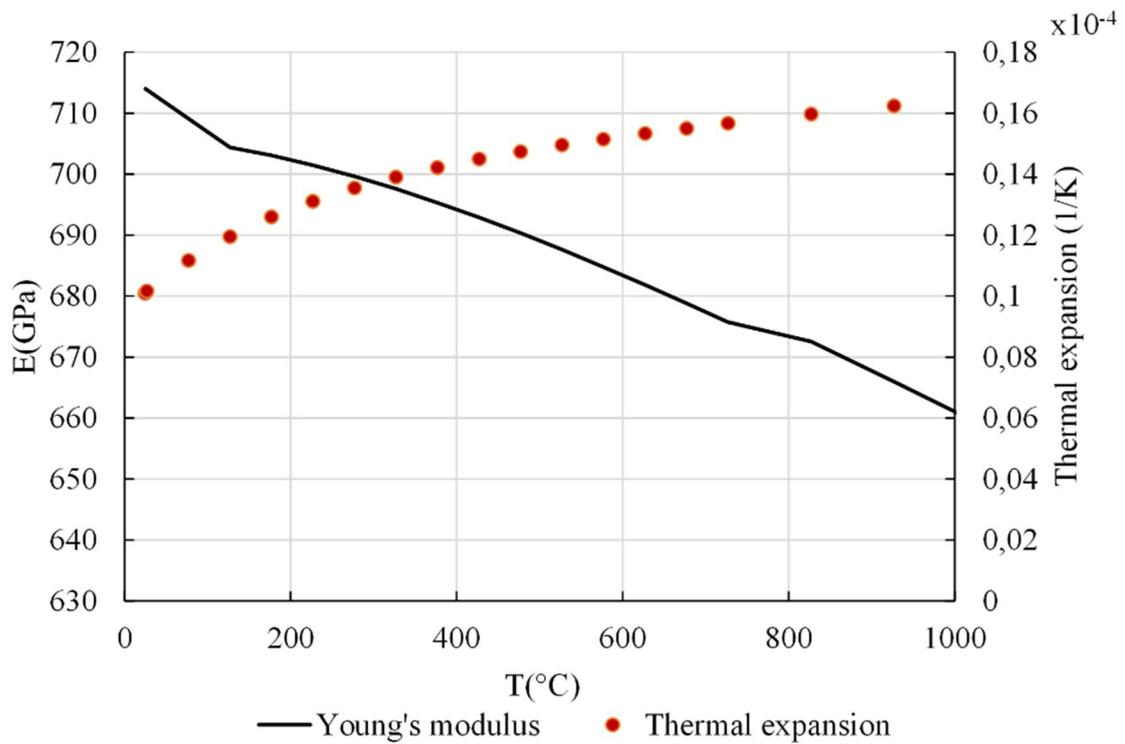
606 **Acknowledgment**

607 The author wishes to thank the French ministry of higher education, research and innovation for
608 financial support.



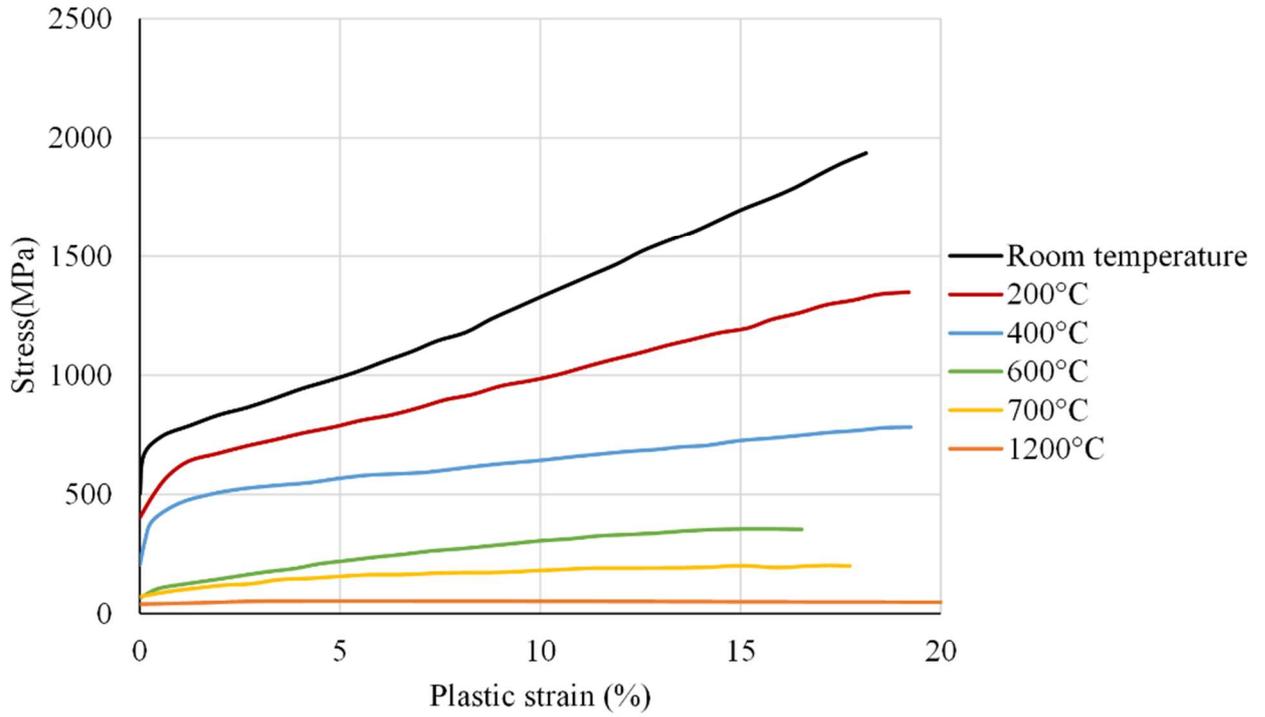
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610 Figure 1. Young's modulus and thermal expansion used for the Co-phase as a function of temperature,
 611 [28, 29].



612

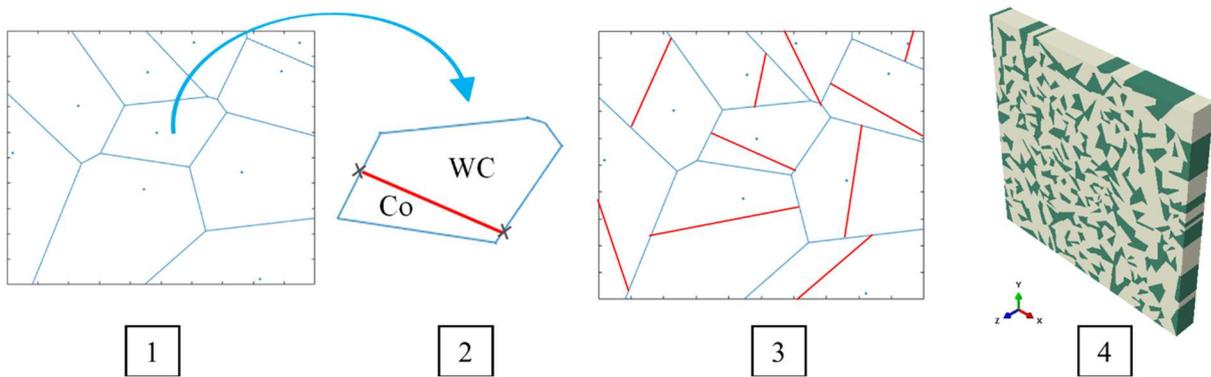
613 Figure 2. Young's modulus and thermal expansion used for the WC-phase as a function of
 614 temperature, [21, 33, 57].



615

616 Figure 3. Stress-plastic strain curves of the Co-phase in uniaxial compression for different

617 temperatures, [38].

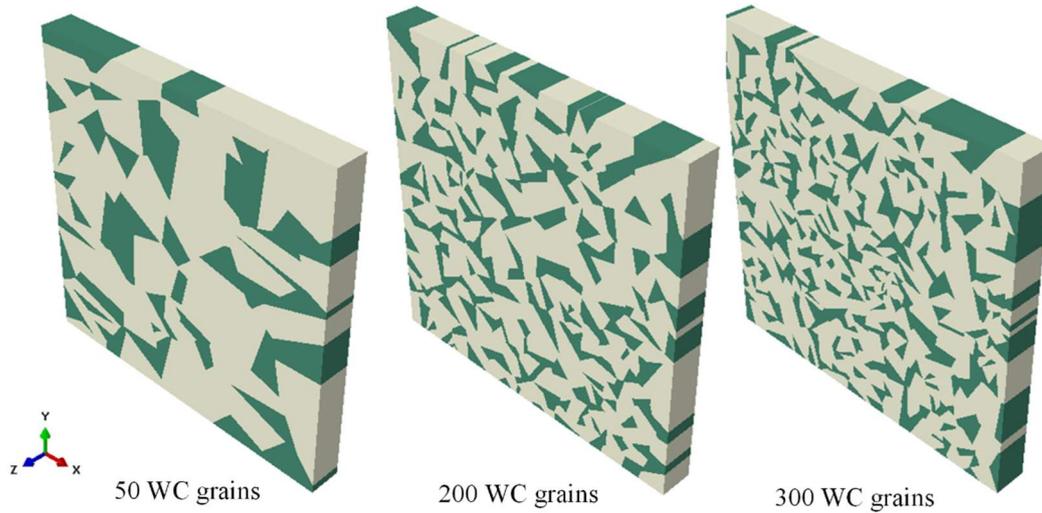


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619 Figure 4. (1) Construction of the Voronoi cells based on random point distribution. (2) Partition of

620 each cell into two phases. (3) Obtained 2D microstructure. (4) Extrusion of the microstructure in the z

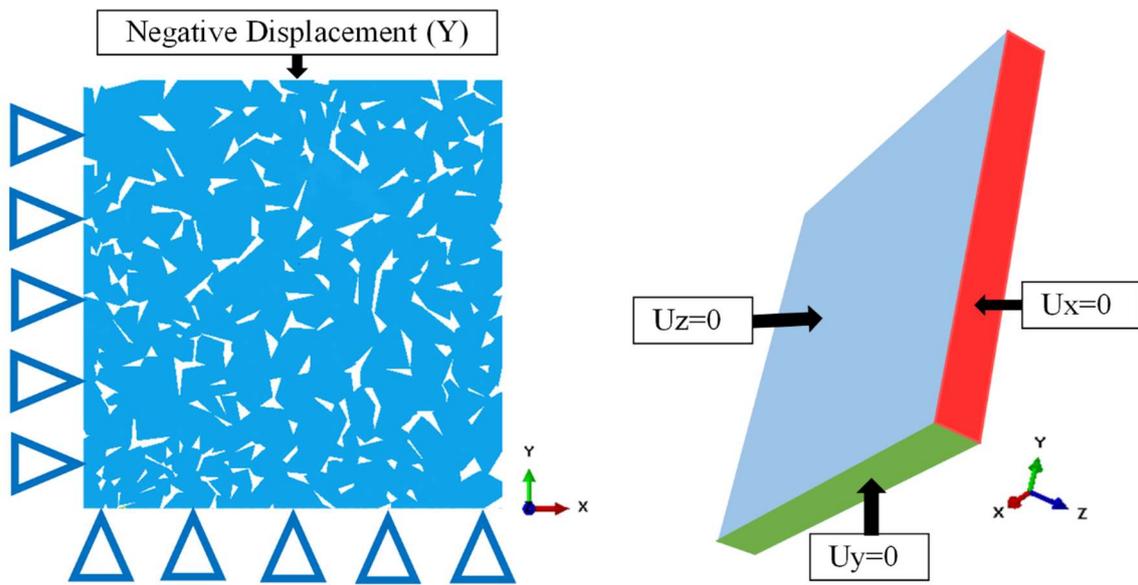
621 direction.



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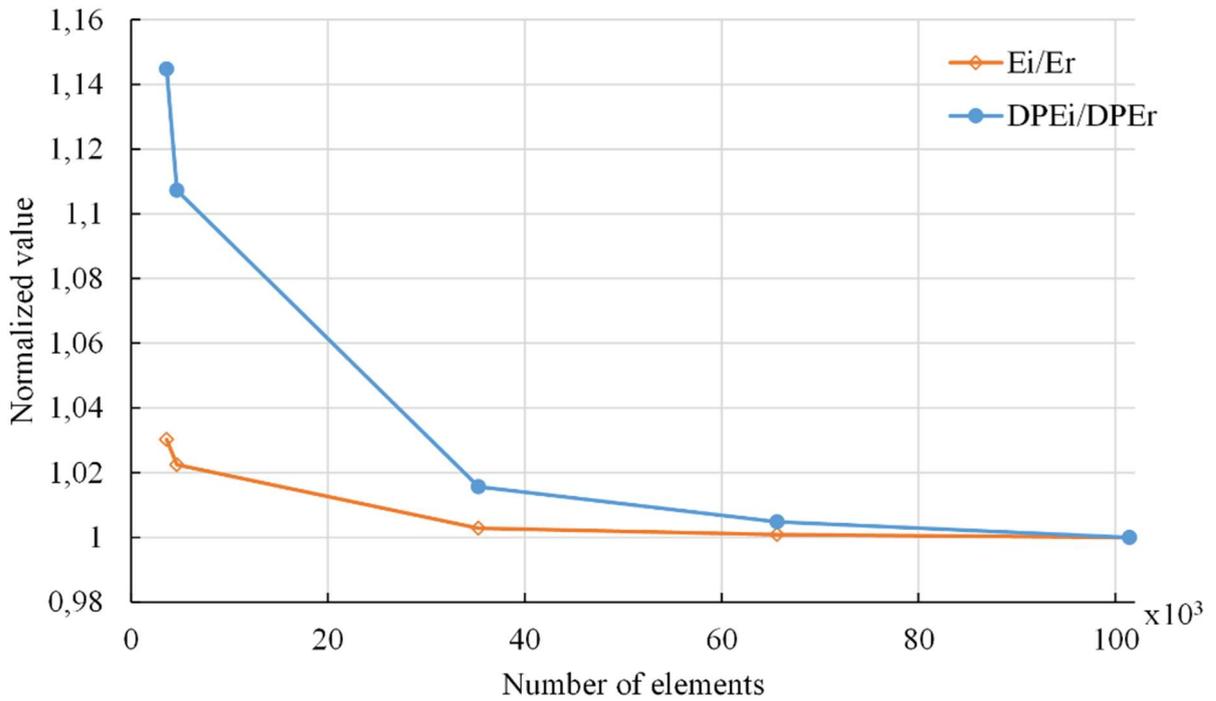
623 Figure 5. Representative elementary volumes with different numbers of WC grains (WC-20wt.%Co).

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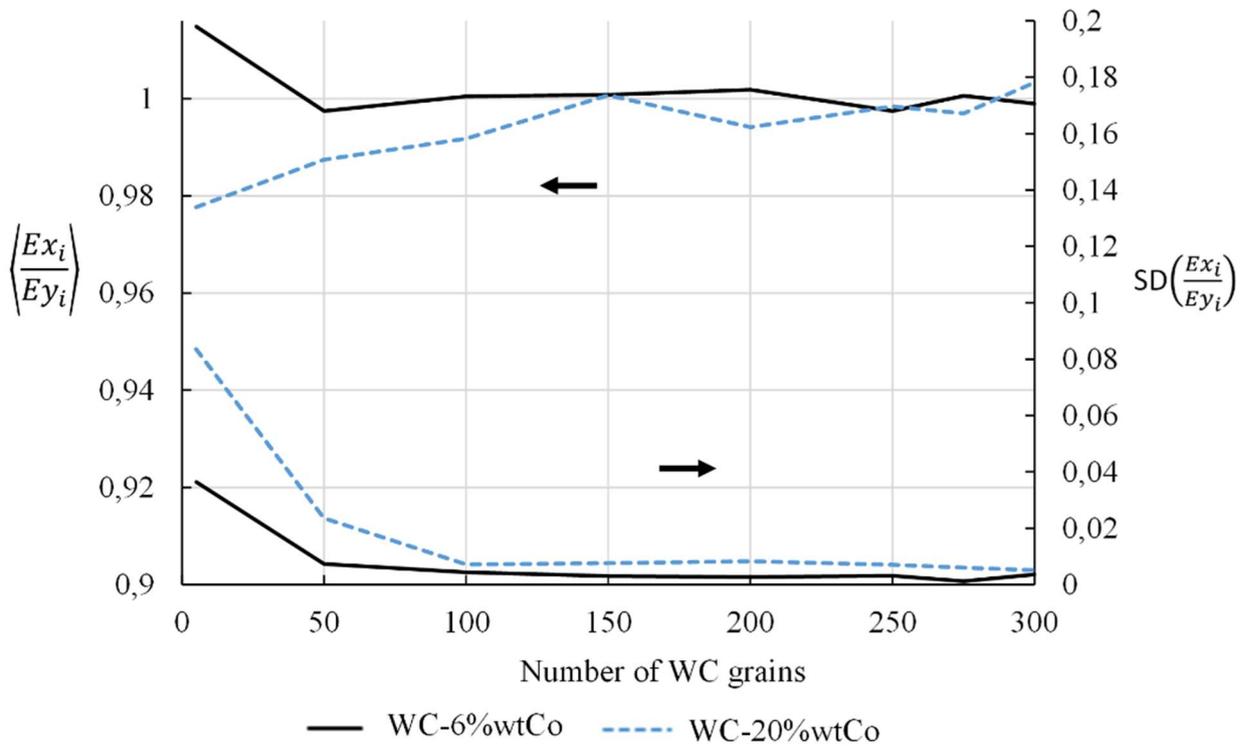
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626 Figure 6. Boundary conditions applied on the RVE. U_x , U_y and U_z are the displacements in x , y and z
 627 directions, respectively.



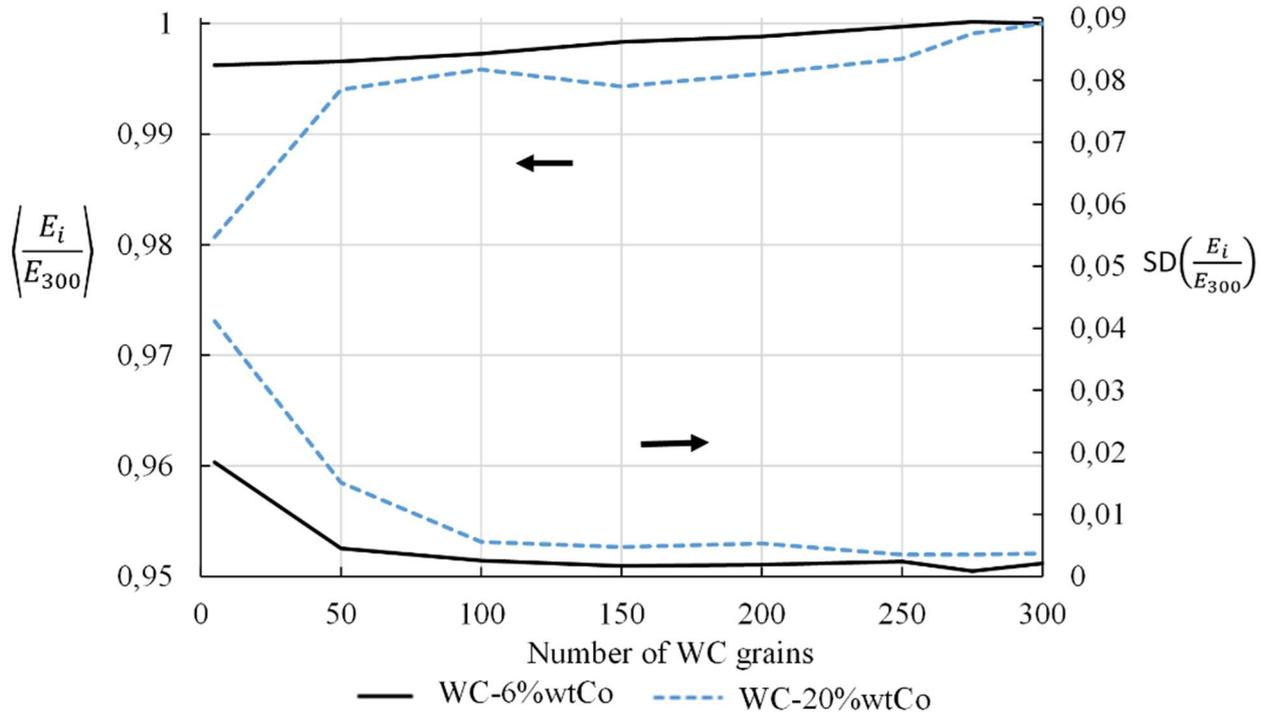
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629 Figure 7. Influence of the number of elements “*i*” on the ratios E_i/E_r and DPE_i/DPE_r . The couples
 630 E_r, E_r and DPE_r, DPE_r are the Young’s moduli and dissipated plastic energies. The r index means
 631 that quantities are computed for 100,000 elements.



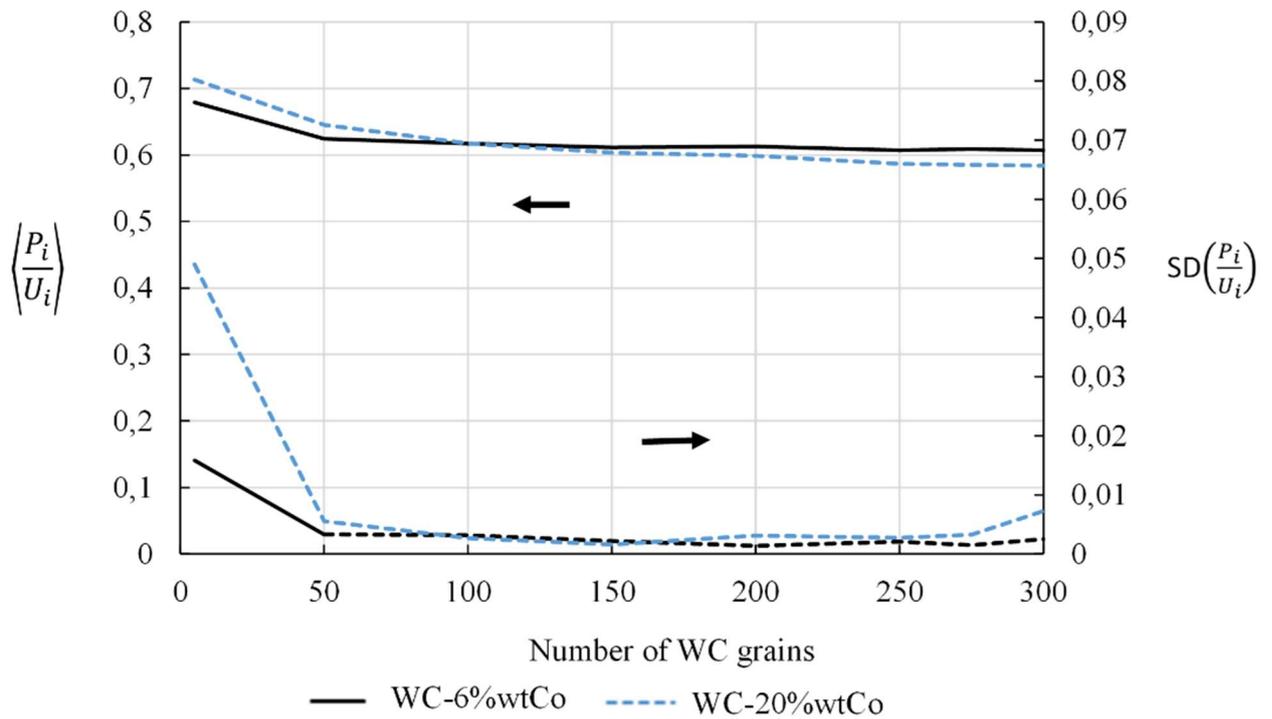
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633 Figure 8. Evolution of the mean ($\langle \rangle$) and standard deviation (SD) of the ratio E_{xi}/E_{yi} as a function of
 634 the WC grains number “ i ”. E_{xi} and E_{yi} are the Young’s moduli computed in the x and y directions for
 635 “ i ” elements, respectively.



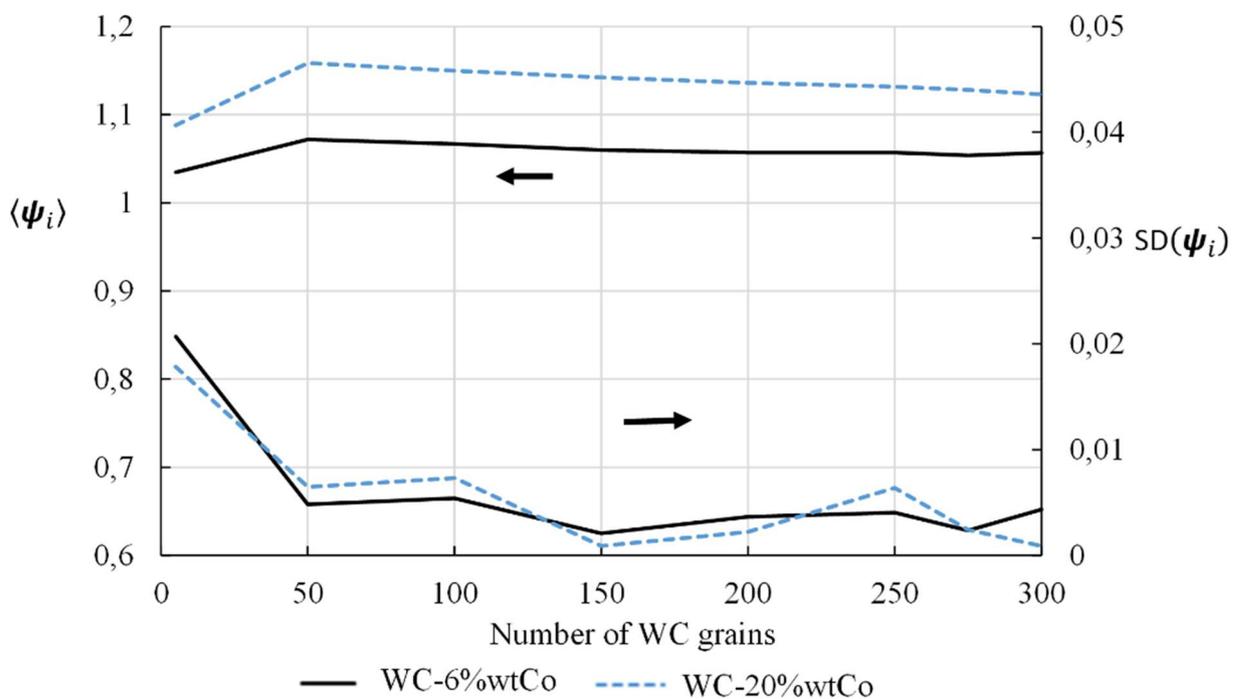
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637 Figure 9. Evolution of the mean ($\langle \rangle$) and standard deviation (SD) of the ratio E_i/E_{300} as a function of
 638 number of WC grains “ i ”. E_i is the Young’s modulus computed for i grains while E_{300} is the mean
 639 Young’s modulus computed for 300 grains.



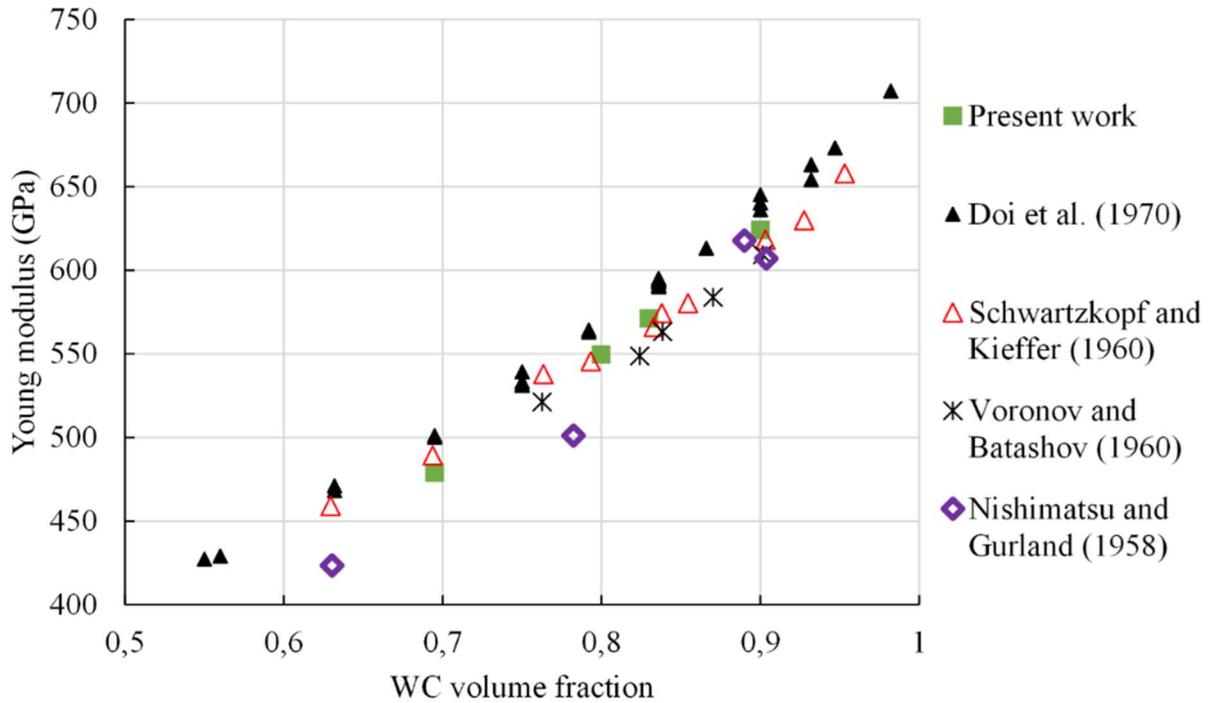
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641 Figure 10. Evolution of the mean ($\langle \rangle$) and standard deviation (SD) of the ratio P_i/U_i as a function of
 642 the number of grains “ i ”. P_i and U_i are the dissipated plastic energy and the external work,
 643 respectively.



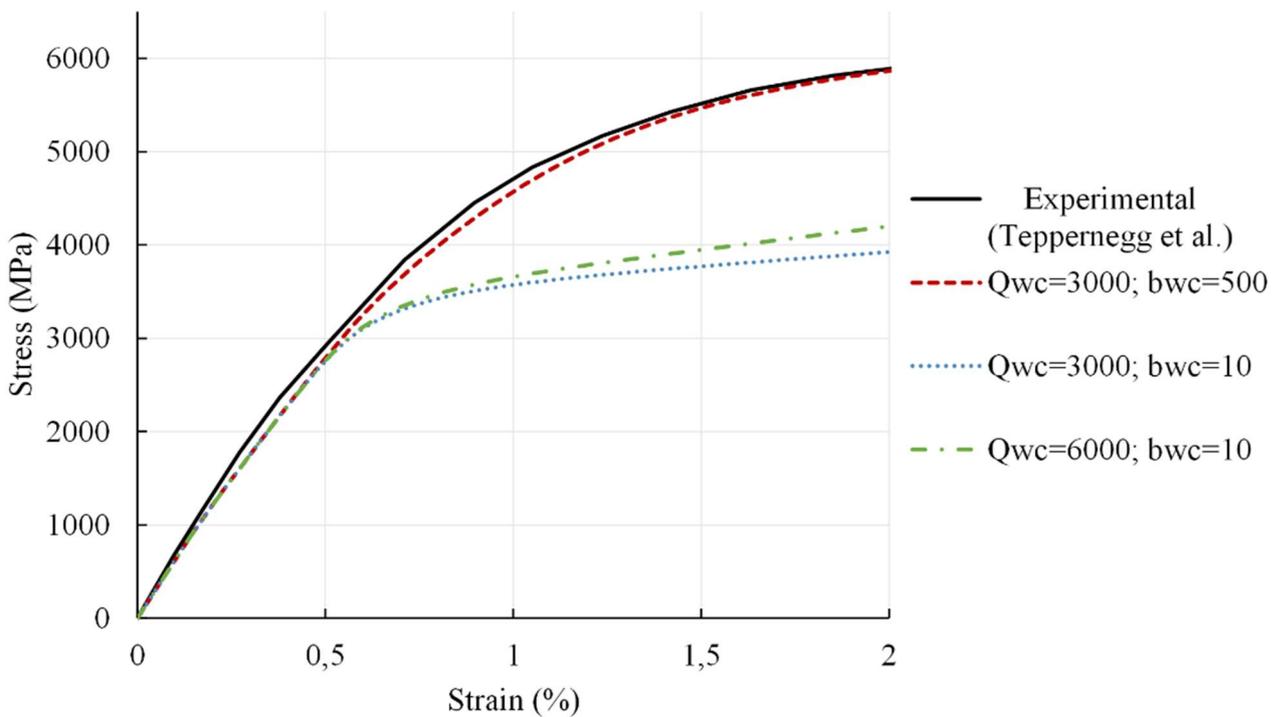
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645 Figure 11. Evolution of the mean ($\langle \rangle$) and standard deviation (SD) of Hill criteria ψ_i as a function of
 646 WC grains “ i ”.



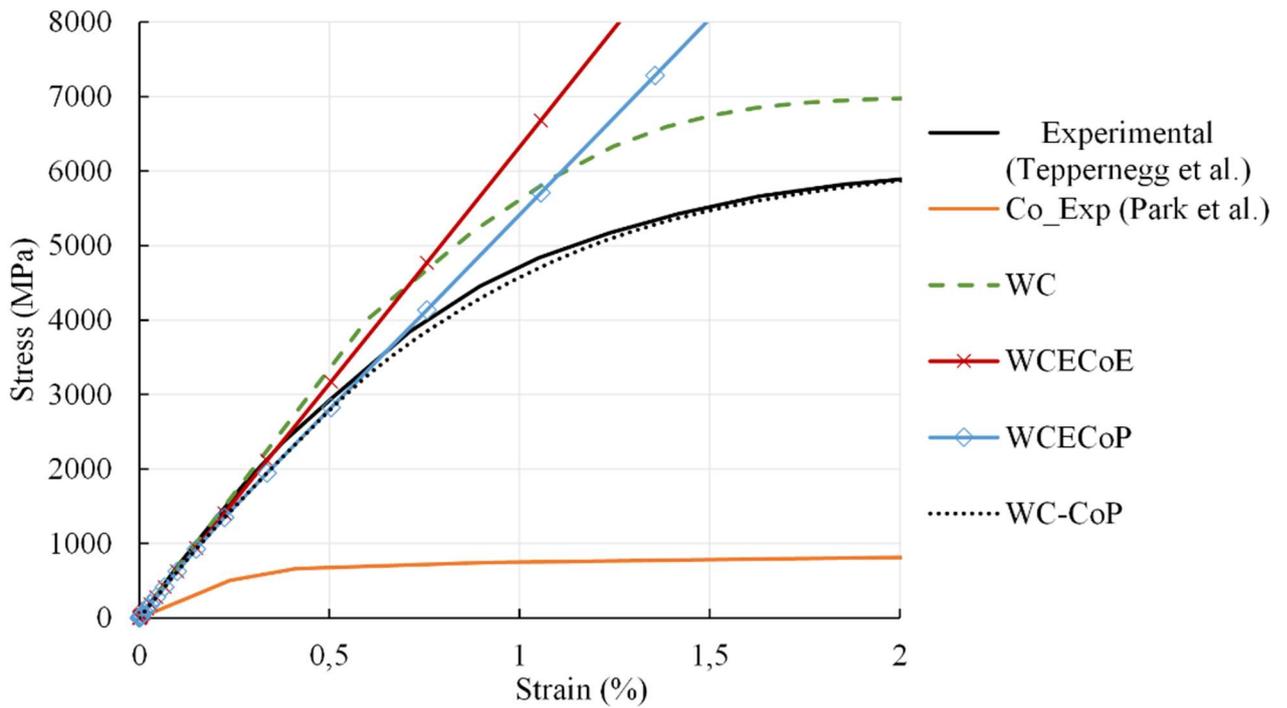
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648 Figure 12. Comparison between the simulated Young's modulus for WC-Co with different WC
 649 volume fractions and experimental results [48–51].



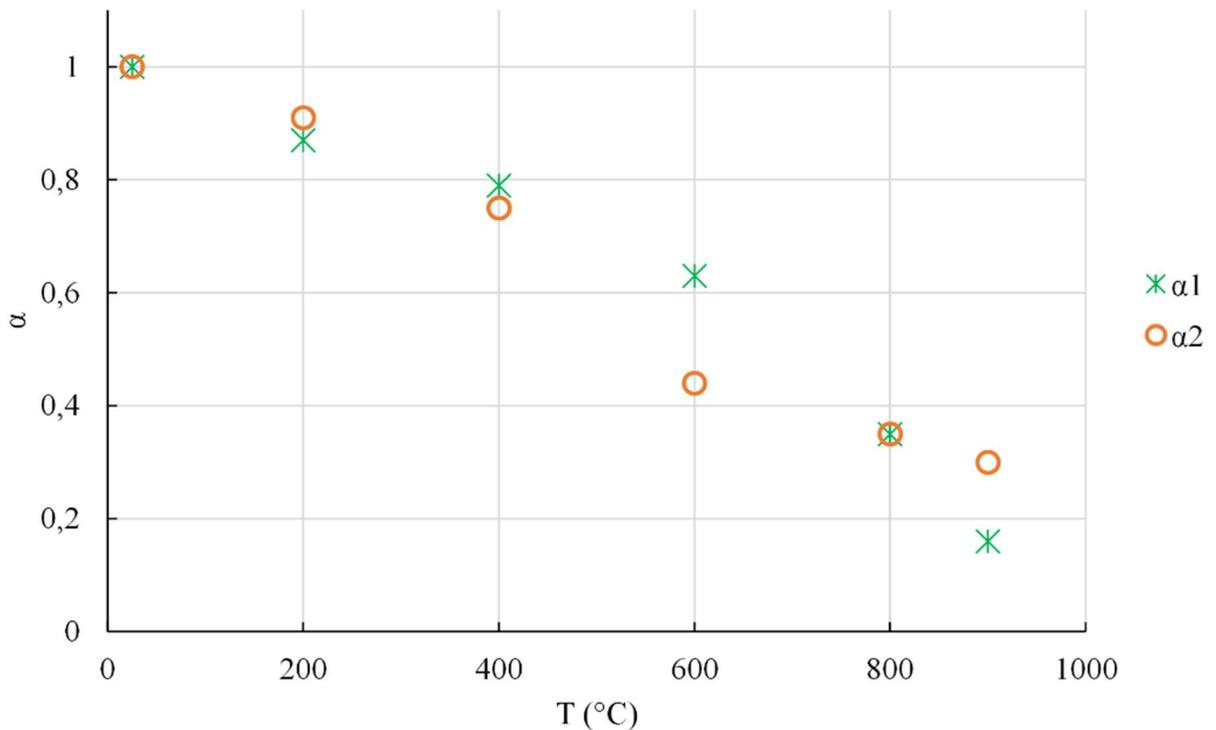
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651 Figure 13. Influence of the hardening parameters Q_{WC} and b_{WC} on the computed stress-strain curves
 652 for a composite WC-6wt.%Co in uniaxial compressive test.



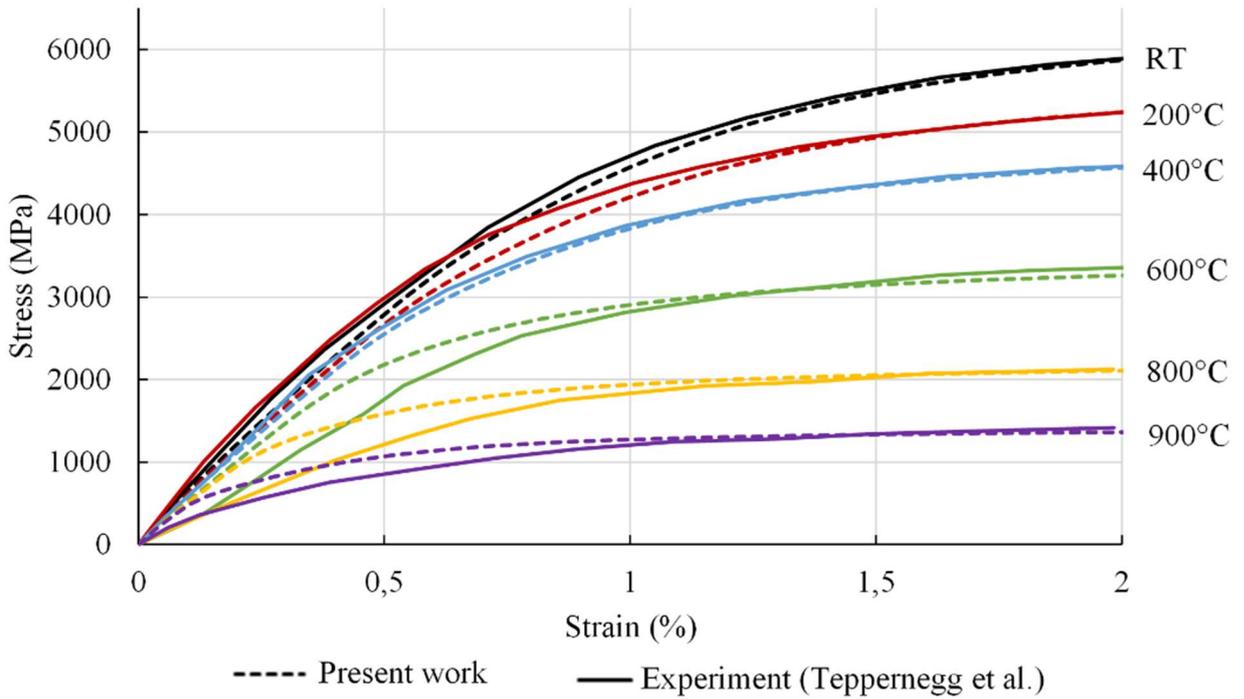
653

654 Figure 14. Comparison between the stress-strain curves for different combinations of phase behaviour
 655 in uniaxial compression with experimental data taken from references [30] and [38]. The indices E and
 656 P mean that the phases have elastic and elasto-plastic behaviours, respectively. For the WC phase, the
 657 selected hardening parameters are $Q_{WC}=3000\text{MPa}$ and $b_{wc}=500$.



658

659 Figure 15. Evolution of α_1 and α_2 parameters as a function of temperature.



660

661 Figure 16. Comparison between experimental results obtained from [30] and computed stress-strain
 662 curves at different temperatures for a composite WC-6wt.%Co under uniaxial compression (200°C-
 663 900°C).

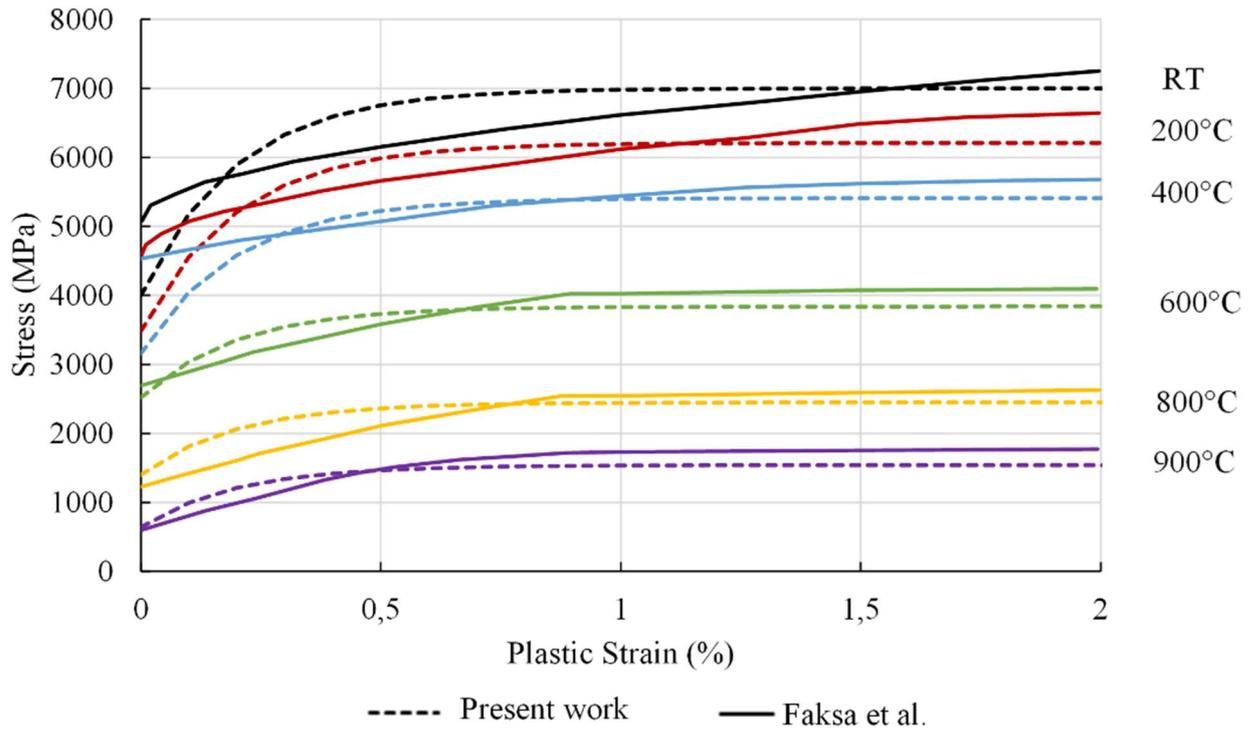
664

665 *Table 1 Summary of the model parameters.*

Cobalt (C_o)		
Young's modulus	E_{C_o}	See Figure 1
Poisson's ratio	ν_{C_o}	0.31 [21]
Coefficient of the thermal expansion	$\alpha_{T C_o}$	See Figure 1
Initial yield stress and hardening		See Figure 3
Tungsten carbide (WC)		
Young's modulus	E_{WC}	See Figure 2
Poisson's ratio	ν_{WC}	0.194 [21]
Coefficient of the thermal expansion	$\alpha_{T WC}$	See Figure 2
Von Mises and Drucker Prager models		
Initial yield stress in uniaxial compression	R_{WC}	4000 MPa [24]
Friction angle	ϕ_{WC}	45°
Dilatation angle	ψ_{WC}	45°
Hardening constants	Q_{WC}	3000 MPa
	b_{WC}	500

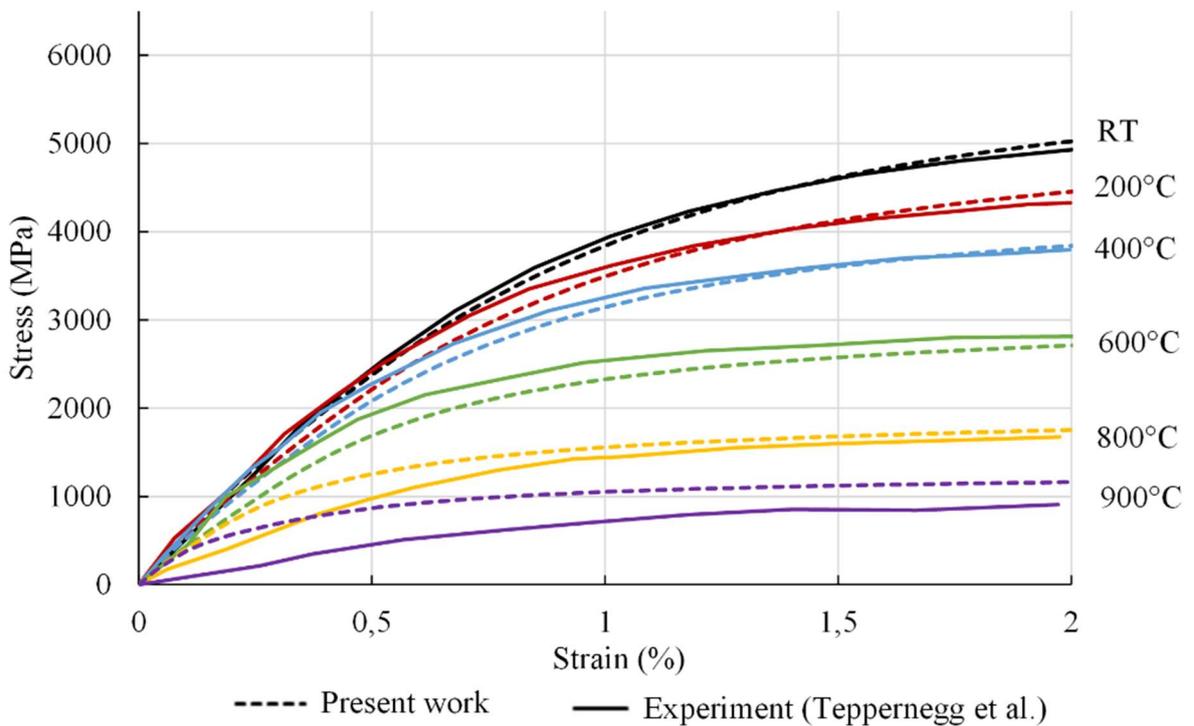
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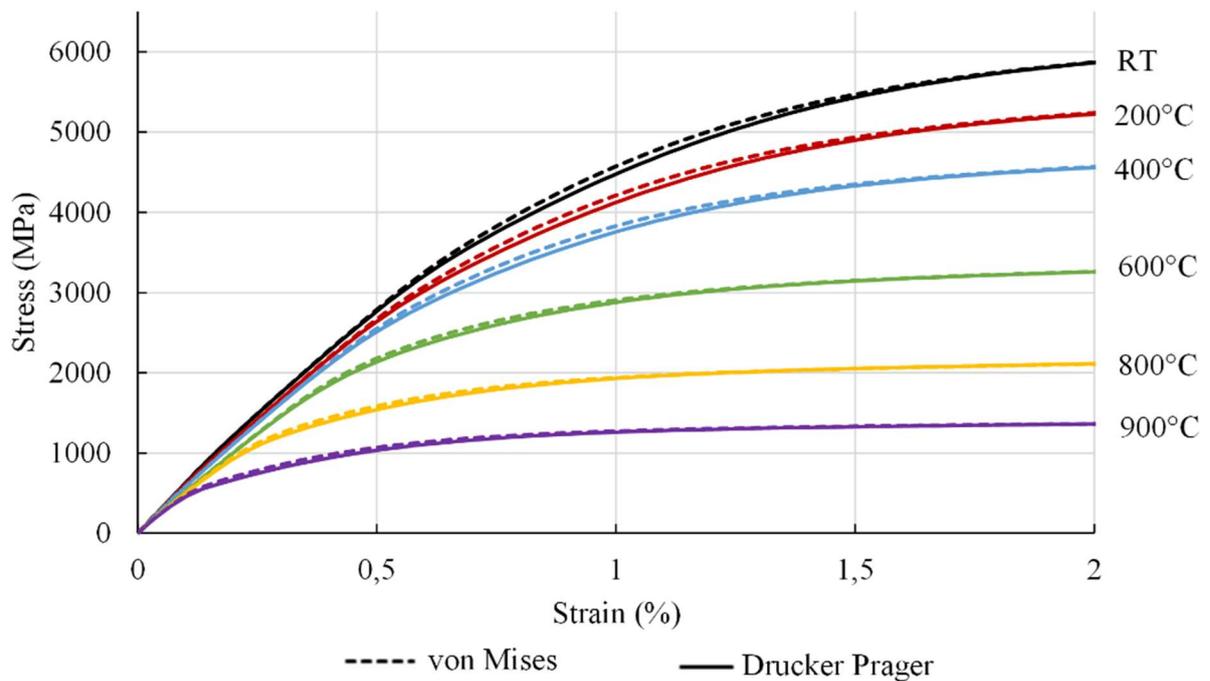
668

669 Figure 17. Comparison between stress-plastic strain curves computed in the present work and by
 670 Faksa et al. [26] for the WC phase for different temperatures (200°C-900°C).



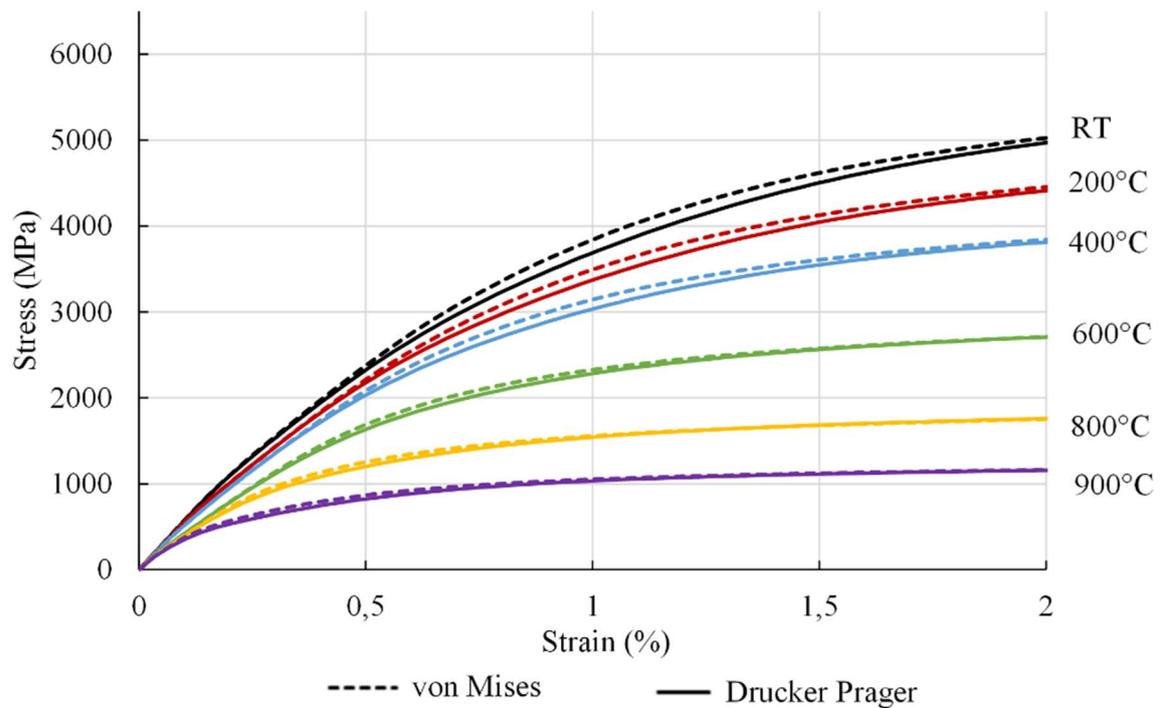
671

672 Figure 18. Comparison between the stress-strain curves computed in the present work and those
 673 measured by Tepperneegg et al. [30] for a composite WC-10.5wt.%Co under uniaxial compression for
 674 different temperatures (200°C-900°C).



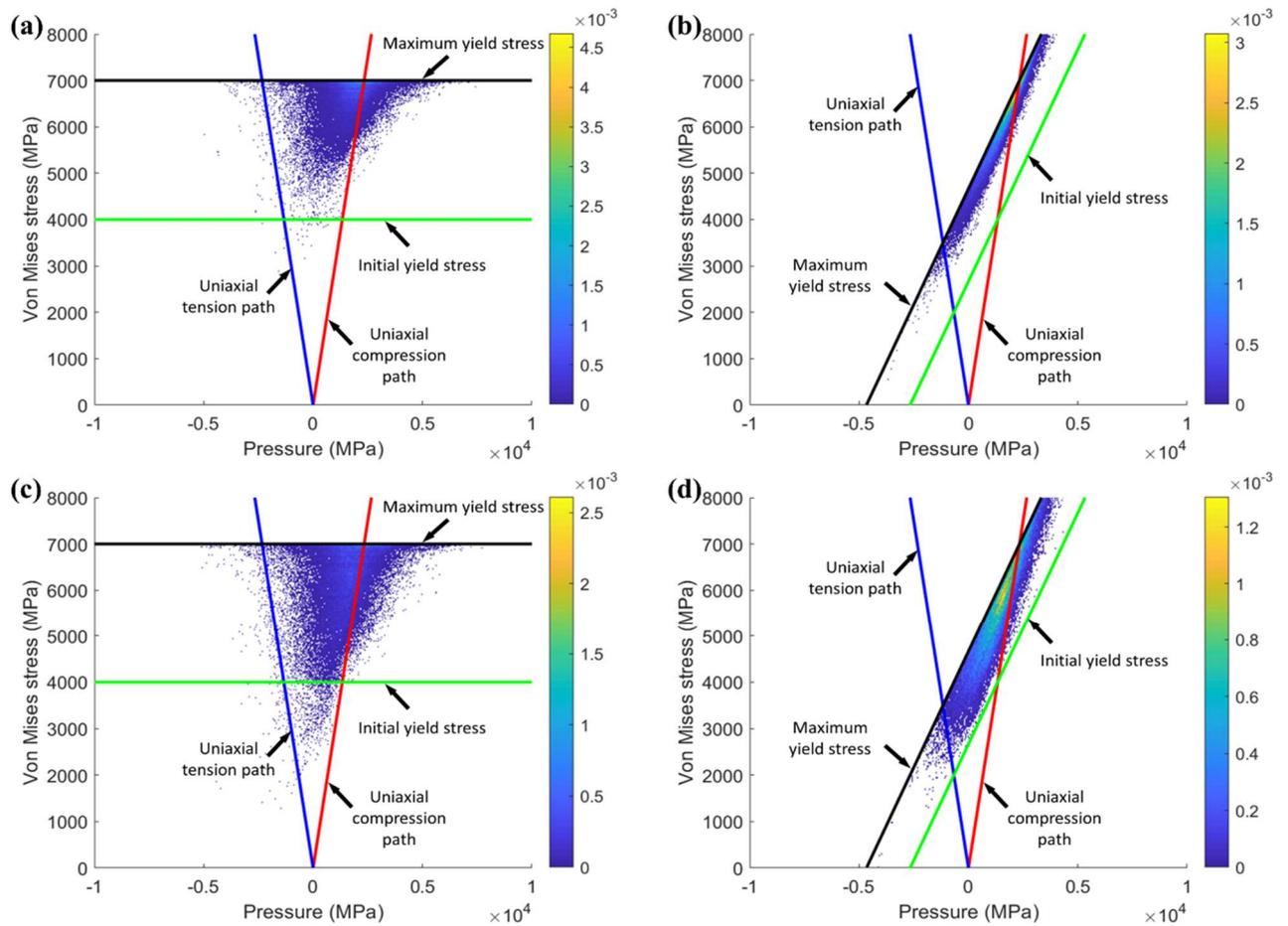
675

676 Figure 19. Comparison between the stress-strain curves computed with von Mises and Drucker Prager
 677 models applied to the tungsten carbide phase for a composite WC-6wt.%Co under uniaxial
 678 compression for different temperatures (200°C-900°C).



679

680 Figure 20. Comparison between the stress-strain curves computed with Mises and Drucker Prager
 681 models applied to the tungsten carbide phase for a composite WC-10.5wt.%Co in uniaxial
 682 compression for different temperatures.



684

685 Figure 21. p-J2 Diagram obtained from the stress tensor calculated at each integration point in the
 686 carbide phase. p is the pressure and J2 the von Mises stress. Each "point" in the figure corresponds to a
 687 rectangle with dimensions of 50x25MPa containing a stress state group. The color of the scale
 688 indicates the probability of finding this stress state group in the carbide phase. These data were
 689 computed with (a): the von Mises criterion and (b): the Drucker Prager criterion for a WC-6wt.%Co
 690 composite, (c): The von Mises criterion and (d) the Drucker Prager criterion for a WC-10.5wt.%Co
 691 composite and for a total strain of 2% at room temperature.

692 **References**

- 693 [1] Z. Z. Fang, M. C. Koopman, and H. Wang, "Cemented Tungsten Carbide Hardmetal-An
694 Introduction," in *Comprehensive Hard Materials*, vol. 1, Elsevier, 2014, pp. 123–137.
- 695 [2] G. Schneider, *Principles of tungsten carbide engineering: Expanded and up-dated to include
696 ceramics*. Society of Carbide and Tool Engineers, 1989.
- 697 [3] H. E. Exner, "Physical and chemical nature of cemented carbides," *Int. Met. Rev.*, vol. 24, no.
698 1, pp. 149–173, 1979, doi: 10.1179/imtr.1979.24.1.149.
- 699 [4] P. E. McHugh and P. J. Connolly, "Micromechanical modelling of ductile crack growth in the
700 binder phase of WC-Co," *Comput. Mater. Sci.*, vol. 27, no. 4, pp. 423–436, 2003, doi:
701 10.1016/S0927-0256(03)00045-4.
- 702 [5] T. Kresse, D. Meinhard, T. Bernthaler, and G. Schneider, "Hardness of WC-Co hard metals:
703 Preparation, quantitative microstructure analysis, structure-property relationship and
704 modelling," *Int. J. Refract. Met. Hard Mater.*, vol. 75, no. May, pp. 287–293, 2018, doi:
705 10.1016/j.ijrmhm.2018.05.003.
- 706 [6] J. García, V. Collado Ciprés, A. Blomqvist, and B. Kaplan, "Cemented carbide
707 microstructures: a review," *Int. J. Refract. Met. Hard Mater.*, vol. 80, no. August 2018, pp. 40–
708 68, 2019, doi: 10.1016/j.ijrmhm.2018.12.004.
- 709 [7] K. S. Ravichandran, "Fracture toughness of two phase WC-Co cermets," *Acta Metall. Mater.*,
710 vol. 42, no. 1, pp. 143–150, 1994, doi: 10.1016/0956-7151(94)90057-4.
- 711 [8] P. Connolly and P. E. McHugh, "Fracture modelling of WC-Co hardmetals using crystal
712 plasticity theory and the Gurson model," *Fatigue Fract. Eng. Mater. Struct.*, vol. 22, no. 1, pp.
713 77–86, 1999, doi: 10.1046/j.1460-2695.1999.00153.x.
- 714 [9] S. Herd, R. J. K. Wood, J. A. Wharton, and C. F. Higgs, "Explicit fracture modelling of
715 cemented tungsten carbide (WC-Co) at the mesoscale," *Mater. Sci. Eng. A*, vol. 712, no. May
716 2017, pp. 521–530, 2018, doi: 10.1016/j.msea.2017.11.109.
- 717 [10] J. T. Smith and J. D. Wood, "Elevated temperature compressive creep behavior of tungsten
718 carbide-cobalt alloys," *Acta Metall.*, vol. 16, no. 10, pp. 1219–1226, 1968.
- 719 [11] F. Ueda, H. Doi, F. Fujiwara, and H. Masatomi, "Bend deformation and fracture of WC-Co
720 alloys at elevated temperatures," *Trans Jpn Inst Met*, vol. 18, no. 3, pp. 247–256, 1977, doi:
721 10.2320/matertrans1960.18.247.

- 722 [12] M. M. Karimi, U. U. Gomes, M. P. Oliveira, R. D. S. Guimarães, M. M. B. Mello, and M.
723 Filgueira, “Fracture toughness evaluation of WC–10 wt% Co hardmetal sintered under high
724 pressure and high temperature,” *High Press. Res.*, vol. 37, no. 1, pp. 59–69, 2017, doi:
725 10.1080/08957959.2016.1261403.
- 726 [13] M. A. Davies, A. L. Cooke, and E. R. Larsen, “High bandwidth thermal microscopy of
727 machining AISI 1045 steel,” *CIRP Ann. - Manuf. Technol.*, vol. 54, no. 1, pp. 63–66, 2005, doi:
728 10.1016/S0007-8506(07)60050-X.
- 729 [14] S. V. Emani, A. F. C. Ramos Dos Santos, L. L. Shaw, and Z. Chen, “Investigation of
730 microstructure and mechanical properties at low and high temperatures of WC-6 wt% Co,” *Int.*
731 *J. Refract. Met. Hard Mater.*, vol. 58, pp. 172–181, 2016, doi: 10.1016/j.ijrmhm.2016.04.009.
- 732 [15] D. Mari, “Déformation à haute température des composites WC-Co,” no. January 1991, 2014,
733 doi: 10.5075/epfl-thesis-938.
- 734 [16] K. H. G. Ashbee, “Intersecting stacking faults in face-centered cubic lattices,” *Acta Metall.*,
735 vol. 15, no. 7, pp. 1129–1131, 1967.
- 736 [17] U. A. Özden, K. Jiang, A. Bezold, and C. Broeckmann, “Evaluation of Fatigue Crack Growth
737 Performance in different Hardmetal Grades based on Finite Element Simulation,” *Procedia*
738 *Struct. Integr.*, vol. 2, pp. 648–655, 2016, doi: 10.1016/j.prostr.2016.06.084.
- 739 [18] H. F. Fischmeister, S. Schmauder, and L. S. Sigl, “Finite element modelling of crack
740 propagation in WC-Co hard metals,” *Mater. Sci. Eng. A*, vol. 105, pp. 305–311, 1988.
- 741 [19] B. O. Jaensson and B. O. Sundström, “Determination of Young’s modulus and poisson’s ratio
742 for WCCo alloys by the finite element method,” *Mater. Sci. Eng.*, vol. 9, no. C, pp. 217–222,
743 1972, doi: 10.1016/0025-5416(72)90036-5.
- 744 [20] B. O. Sundstrom, “Elastic-Plastic Behaviour of WC-Co Analysed by Continuum Mechanics,”
745 vol. 12, 1973.
- 746 [21] M. H. Poech, H. F. Fischmeister, D. Kaute, and R. Spiegler, “FE-modelling of the deformation
747 behaviour of WC-Co alloys,” *Comput. Mater. Sci.*, vol. 1, no. 3, pp. 213–224, 1993, doi:
748 10.1016/0927-0256(93)90013-D.
- 749 [22] T. Sadowski and T. Nowicki, “Numerical investigation of local mechanical properties of
750 WC/Co composite,” *Comput. Mater. Sci.*, vol. 43, no. 1, pp. 235–241, 2008, doi:
751 10.1016/j.commatsci.2007.07.030.
- 752 [23] G. Chen, U. A. Ozden, A. Bezold, and C. Broeckmann, “A statistics based numerical

- 753 investigation on the prediction of elasto-plastic behavior of WC-Co hard metal,” *Comput.*
754 *Mater. Sci.*, vol. 80, pp. 96–103, 2013, doi: 10.1016/j.commatsci.2013.04.004.
- 755 [24] D. Tkalich, G. Cailletaud, V. A. Yastrebov, and A. Kane, “A micromechanical constitutive
756 modeling of WC hardmetals using finite-element and uniform field models,” *Mech. Mater.*,
757 vol. 105, pp. 166–187, 2017, doi: 10.1016/j.mechmat.2016.11.007.
- 758 [25] D. Tkalich, V. A. Yastrebov, G. Cailletaud, and A. Kane, “Multiscale modeling of cemented
759 tungsten carbide in hard rock drilling,” *Int. J. Solids Struct.*, vol. 128, pp. 282–295, 2017, doi:
760 10.1016/j.ijsolstr.2017.08.034.
- 761 [26] L. Faksa *et al.*, “Shot peening-induced plastic deformation of individual phases within a coated
762 WC-Co hard metal composite material including stress-strain curves for WC as a function of
763 temperature,” *Surf. Coatings Technol.*, vol. 380, no. September, p. 125026, 2019, doi:
764 10.1016/j.surfcoat.2019.125026.
- 765 [27] J. Weidow and H. O. Andrén, “Binder phase grain size in WC-Co-based cemented carbides,”
766 *Scr. Mater.*, vol. 63, no. 12, pp. 1165–1168, 2010, doi: 10.1016/j.scriptamat.2010.08.025.
- 767 [28] W. Betteridge, “The properties of metallic cobalt,” *Prog. Mater. Sci.*, vol. 24, no. C, pp. 51–
768 142, 1980, doi: 10.1016/0079-6425(79)90004-5.
- 769 [29] M. E. Fine and W. C. Ellis, “Thermal expansion properties of iron-cobalt alloys,” *Trans. Am.*
770 *Inst. Min. Met. Eng.*, vol. 175, p. 742, 1948.
- 771 [30] T. Tepperneegg *et al.*, “High temperature mechanical properties of WC-Co hard metals,” *Int. J.*
772 *Refract. Met. Hard Mater.*, vol. 56, pp. 139–144, 2016, doi: 10.1016/j.ijrmhm.2016.01.002.
- 773 [31] J. fei Zhu, L. Zhang, H. dong Zhang, Z. qiang Zhong, L. Zhou, and Y. Chen, “Real
774 microstructure-based simulation of thermal residual stresses in cemented carbides and the
775 related strengthening and toughening consideration,” *Int. J. Refract. Met. Hard Mater.*, vol. 71,
776 no. November 2017, pp. 239–245, 2018, doi: 10.1016/j.ijrmhm.2017.11.014.
- 777 [32] T. Sadowski, S. J. Hardy, and E. W. Postek, “Prediction of the mechanical response of
778 polycrystalline ceramics containing metallic intergranular layers under uniaxial tension,”
779 *Comput. Mater. Sci.*, vol. 34, no. 1, pp. 46–63, 2005, doi: 10.1016/j.commatsci.2004.10.005.
- 780 [33] R. R. Reeber and K. Wang, “Thermophysical Properties of Tungsten Carbide,” vol. 35, 1999.
- 781 [34] T. Takahashi and E. J. Freise, “Determination of the slip systems in single crystals of tungsten
782 monocarbide,” *Philos. Mag.*, vol. 12, no. 115, pp. 1–8, 1965, doi:
783 10.1080/14786436508224941.

- 784 [35] M. K. Hibbs and R. Sinclair, "Room-temperature deformation mechanisms and the defect
785 structure of tungsten carbide," *Acta Metall.*, vol. 29, no. 9, pp. 1645–1654, 1981.
- 786 [36] V. K. Sarin and T. Johannesson, "On the deformation of WC--Co cemented carbides," *Met.*
787 *Sci.*, vol. 9, no. 1, pp. 472–476, 1975.
- 788 [37] V. Abaqus, "6.14 Documentation," *Dassault Syst. Simulia Corp.*, vol. 651, pp. 2–6, 2014.
- 789 [38] S. Park, S. G. Kapoor, and R. E. DeVor, "Microstructure-level model for the prediction of tool
790 failure in WC-Co cutting tool materials," *J. Manuf. Sci. Eng.*, vol. 128, no. 3, pp. 739–748,
791 2006.
- 792 [39] D. C. Drucker and W. Prager, "Soil mechanics and plastic analysis or limit design," *Q. Appl.*
793 *Math.*, vol. 10, no. 2, pp. 157–165, 1952.
- 794 [40] H. Doi, *Elastic and Plastic Properties of WC-Co Composite Alloys*. Freund Publishing House,
795 1974.
- 796 [41] M. Christensen and G. Wahnström, "Effects of cobalt intergranular segregation on interface
797 energetics in WC-Co," *Acta Mater.*, vol. 52, no. 8, pp. 2199–2207, 2004, doi:
798 10.1016/j.actamat.2004.01.013.
- 799 [42] T. Csanádi, M. Vojtko, and J. Dusza, "Deformation and fracture of WC grains and grain
800 boundaries in a WC-Co hardmetal during microcantilever bending tests," *Int. J. Refract. Met.*
801 *Hard Mater.*, vol. 87, no. July 2019, p. 105163, 2020, doi: 10.1016/j.ijrmhm.2019.105163.
- 802 [43] W. Dawihl and J. Hinnüber, "Über den Aufbau der Hartmetalllegierungen," *Kolloid-Zeitschrift*,
803 vol. 104, no. 2, pp. 233–236, Sep. 1943, doi: 10.1007/BF01519451.
- 804 [44] E. Jiménez-Piqué *et al.*, "Focused ion beam tomography of WC-Co cemented carbides," *Int. J.*
805 *Refract. Met. Hard Mater.*, vol. 67, no. April, pp. 9–17, 2017, doi:
806 10.1016/j.ijrmhm.2017.04.007.
- 807 [45] G. List, "Etude des mécanismes d'endommagement des outils carbure WC-Co par la
808 caractérisation de l'interface outil copeau: application à l'usinage à sec de l'alliage
809 d'aluminium aéronautique AA2024 T351," Paris, ENSAM, 2004.
- 810 [46] W. Kayser, A. Bezold, and C. Broeckmann, "Simulation of residual stresses in cemented
811 carbides," *Int. J. Refract. Met. Hard Mater.*, vol. 63, pp. 55–62, 2017, doi:
812 10.1016/j.ijrmhm.2016.04.001.
- 813 [47] E. Postek and T. Sadowski, "Dynamic pulse sensitivity of WC/Co composite," *Compos.*

- 814 *Struct.*, vol. 203, no. July 2017, pp. 498–512, 2018, doi: 10.1016/j.compstruct.2017.10.092.
- 815 [48] P. Schwarzkopf and R. Kieffer, *Cemented carbides*. Macmillan, 1960.
- 816 [49] F. Voronov and D. Balashov, “The adiabatic moduli of elasticity in sintered tungsten carbide
817 cutting alloys,” *Phys. Met. Met.*, vol. 9, no. 4, pp. 127–130, 1960.
- 818 [50] C. Nishimatsu and J. Gurland, “Experimental survey of the deformation of a hard-ductile two-
819 phase alloy system (WC-CO),” 1958.
- 820 [51] H. Doi, Y. Fujiwara, K. Miyake, and Y. Oosawa, “A systematic investigation of elastic moduli
821 of Wc-Co alloys,” *Metall. Mater. Trans.*, vol. 1, no. 5, pp. 1417–1425, 1970, doi:
822 10.1007/BF02900264.
- 823 [52] N. Hansen, “Hall-petch relation and boundary strengthening,” *Scr. Mater.*, vol. 51, no. 8 SPEC.
824 ISS., pp. 801–806, 2004, doi: 10.1016/j.scriptamat.2004.06.002.
- 825 [53] F. De Luca *et al.*, “Nanomechanical Behaviour of Individual Phases in WC-Co Cemented
826 Carbides, from Ambient to High Temperature.,” *Materialia*, vol. 12, no. May, 2020, doi:
827 10.1016/j.mtla.2020.100713.
- 828 [54] M. A. Yousfi, J. Weidow, A. Nordgren, L. K. L. Falk, and H. O. Andrén, “Deformation
829 mechanisms in a WC-Co based cemented carbide during creep,” *Int. J. Refract. Met. Hard
830 Mater.*, vol. 49, no. 1, pp. 81–87, 2015, doi: 10.1016/j.ijrmhm.2014.07.016.
- 831 [55] T. Csanádi, M. Břanda, A. Duszová, N. Q. Chinh, P. Szommer, and J. Dusza, “Deformation
832 characteristics of WC micropillars,” *J. Eur. Ceram. Soc.*, vol. 34, no. 15, pp. 4099–4103, 2014,
833 doi: 10.1016/j.jeurceramsoc.2014.05.045.
- 834 [56] T. Sakuma and H. Hondo, “Plastic flow in WC-13wt.%Co at high temperatures,” *Mater. Sci.
835 Eng. A*, vol. 156, no. 2, pp. 125–130, 1992, doi: 10.1016/0921-5093(92)90144-P.
- 836 [57] W. Koster, “The Temperature Dependence of the Elastic Modulus of Pure Metals,” *Ztsch. für
837 Met.*, vol. 39, p. 1, 1948.

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