Cover letter

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To
Editor, Materials and Metallurgical Transactions A

From
Dr. Anish Upadhyaya
Professor
Department of Materials Science and Engineering
Indian Institute of Technology Kanpur 208016 UP
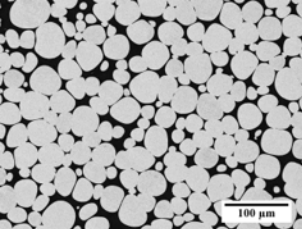anishu@iitk.ac.in

Dear Sir,

We wish to submit an original research article entitled "Texture evolution during uniaxial compression of tungsten heavy alloys" for consideration for publication as regular article in your journal. This paper is based on the doctoral research work carried out by the co-author Mr. Mirtunjay Kumar in our guidance (Drs. NP Gurao and A. Upadhyaya). On behalf of all the coauthors, I confirm that this work is original and has not been published elsewhere, nor is it currently under consideration for publication elsewhere.

This paper investigated the crystallographic texture evolution of tungsten heavy alloy in compression load. This study is significant because WHA undergoes a large deformation upon ballistic impact. So, a systematic investigation of the deformation of this heavy alloy is needed. As crystallographic texture evolution during processing plays a vital role in the mechanical behaviour of the alloy, we compressed the W-Ni-Fe heavy alloy where tungsten content varied from 80 to 98 and captured the texture with macro and micro-texture measurements. In order to understand the evolved texture, the initial texture was modelled with the appropriate model using VPSC, and the micro-mechanism related to texture evolution has been demonstrated.
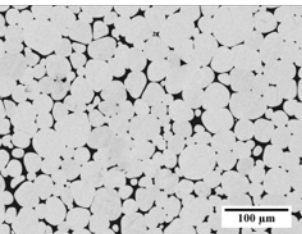
We believe this manuscript is appropriate for publication in MMTA. We have no conflicts of interest to disclose. Any correspondence related to the manuscript may kindly be communicated to me at anishu@iitk.ac.in.
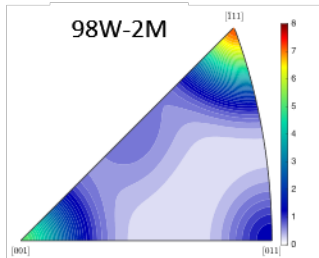
Sincerely,

Anish Upadhyaya

80W-20M

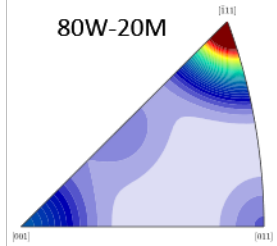98W-2M

Load

Sample

80W-20M

98W-2M

True stress, MPa

True strain

- 80W
- 85W
- 90W
- 95W
- 98W

Work hardening rate (dσ/dε) ×10³, MPa

$\sigma - \sigma_0$, MPa

- 80W
- 85W
- 90W
- 95W
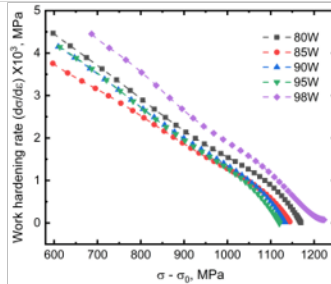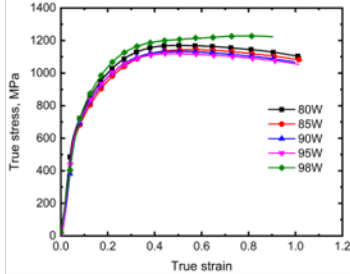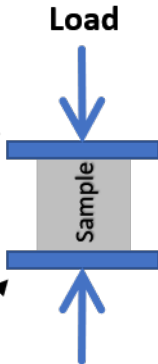- 98W

Effect of Tungsten Content and Compression on Microstructure and Texture Evolution in Liquid Phase Sintered Heavy Alloy

Mirtunjay Kumar, N.P. Gurao, Anish Upadhyaya*

Department of Materials Science and Engineering,
Indian Institute of Technology Kanpur 208016 INDIA

[*] corresponding author: anishu@iitk.ac.in

Abstract:

The crystallographic texture development in uniaxial compression tests of tungsten heavy alloys was systematically investigated by varying the tungsten content of the alloys. It was observed that a characteristic double fiber texture consisting of <111> and <100> fibers in the b.c.c. tungsten particles, regardless of the alloy composition under consideration. The effect of the composition was shown mainly in relation to the relative proportion of <100> and <111> fiber. It was observed that the <100> fiber strengthens with increasing tungsten content, although the <111> fiber remained as the strongest fiber in all the five compositions considered in the present work. The strengthening of <100> fibers with an increased tungsten content was understood by performing self-consistent texture simulations in combination with a lattice corotation scheme to account for the role of neighboring grain orientations in texture evolution. A physical justification of the role of the neighbors is given by the shift of the orientations around the [110]-[411] divergent line. The random fluctuations that originate from the neighbors displaces the orientation from the above of divergent downwards, which in turn leads to the displaced grains rotating in the direction of the <100> corner.

Keywords: Tungsten heavy alloys; Texture; VPSC

1. Introduction

Tungsten Heavy Alloys (WHA) are widely used as kinetic-energy penetrators (KEP), vibration dampers, counterweights and medical radiation protection devices, due to their unique combination of characteristics such as high density (16-18 g/cm^3) and strength (1000-1700 MPa), reasonably ductile (10-30%), excellent corrosion resistance and easy machinability [1]. Depleted uranium alloys have traditionally been used as KEP materials. However, because of their environmental and health concerns, there is a need to replace these alloys with an alternative material [2]. WHA are the most promising alloys in this regard and have therefore received a great deal of attention from many researchers in the past. Although the properties of WHAs are very promising, they lack a self-sharpening effect, which in turn leads to the formation of mushroom head on impact [3]. Much effort has been made to strategically process the WHA to enhance the ballistic performance of WHA through tailoring the composition [4,5], heat treatment [6] and manufacturing methods such as solid-state sintering [7], liquid phase sintering [8], spark plasma sintering [9], microwave sintering [10], electrodeposition [11], laser melting deposition [12] and selective laser melting [13].

The WHA are mainly produced by powder metallurgy using liquid phase sintering (LPS). These composites typically contain 80-98 wt% W along with transition metals such as Ni, Fe, Cu and Co, etc. WHA with a tungsten content of less than 80% by weight leads to slumping during sintering and microstructural inhomogeneities and is therefore generally not used for commercial applications [14]. The microstructure of these alloys can be characterized by the presence of rounded tungsten grains dispersed in a low melting point ductile matrix phase. The microstructural properties of WHA, such as the grain size of tungsten particles, connectivity (average two-dimensional coordination number of tungsten particles), contiguity (relative proportion of the tungsten-tungsten interface in relation to the total interface) and

53 volume fraction of matrix, play an important role in controlling the deformation behavior

54 [15,16].

55   Much research has been done in the past to investigate the mechanical properties and

56 microstructure evolution of WHAs over the past few decades [17–19]. Jinglian et al. [20]

57 examined the WHA with fine particle size and showed the better mechanical properties and

58 the development of early shear band formation. Das et al. [21] showed that these alloys can

59 withstand up to 70% of deformation without cracking even at 400°C. The deformation

60 behavior also depends on the strain rate and the temperature and flow stress increases with

61 increasing strain rate and decreasing test temperature [22,23]. Significant flow softening was a

62 characteristic observation when the grain size of the alloy was reduced to a few micrometers

63 [24]. Yu et al. [25,26] and Zhang et al. [25,26] investigated the hot extrusion of WHA alloys, which

64 led to an improvement in ultimate tensile strength and hardness but a decrease in ductility.

65   In practice, the WHA alloys are mainly subjected to compression deformation.

66 Therefore, most of the work in earlier studies has focused on understanding the deformation

67 behavior under compression in relation to the mechanical properties (work hardening rate,

68 strain rate sensitivity) [27]. However, the evolution of the crystallographic texture during

69 uniaxial compression tests was not taken into account. It is known that the mechanical

70 properties are considerably dependent on the crystallographic texture [28]. It was shown that an

71 improvement in the mechanical properties can be achieved through suitable texture

72 engineering. The relationship between processing, texture and mechanical properties is also

73 missing in WHA for different phase fractions of tungsten. Therefore, it is of the utmost

74 importance to systematically study the texture evolution during the uniaxial compression of

75 WHA in order to understand the governing deformation mechanism. The texture evolution of

76 single-phase b.c.c. has been extensively investigated by many researchers in the past [29,30].

77 However, very little information is available for two-phase alloys, particularly for WHA.

78 In this context, the aim of the present work is to carry out texture measurements of WHAs

79 after uniaxial compression tests in order to understand the deformation behaviour. In addition

80 to the microstructural characterization, to supplement the texture measurements, simulation

81 studies with viscoplastic self-consistent simulations are carried out.

82

83 **2. Experimental Details**

84 In the present work, elemental powders with a purity of 99.99% were used as raw

85 material for the synthesis of W-Ni-Fe based WHA. The composition of the WHA and the

86 corresponding sample nomenclatures are listed in Table 1. The powders were mixed in a

87 stoichiometric ratio and compacted into a cylindrical shape using hydraulic press at 300 MPa.

88 **Table 1** Composition of tungsten heavy alloy.

Alloy	W (wt.%)	Ni (wt.%)	Fe (wt.%)
80W-20M	80	14	6
85W-15M	85	10.5	4.5
90W-10M	90	7	3
95W-5M	95	3.5	1.5
98W-2M	98	1.4	0.6

89

90 The tungsten compact was then sintered in a tube furnace at 1773 K for 1 hour under a

91 flowing hydrogen atmosphere. A sintered alloy was obtained which consisted of coarse

92 tungsten particles surrounded by a completely wet matrix phase.

93 The sintered composites were then cut into cylindrical samples (Ø6 mm × 4.8 mm),

94 having a length to diameter ratio of 0.8 [31] for performing uniaxial compression testing using

95 a universal testing machine (Biss India Pvt Ltd). The strain rate used during the compression

96 tests was kept at 10^{-3} s^{-1}. The compression tests were performed up to a true strain (ε) of

97   0.693, which corresponds to a 50% reduction in height. The compression tests were repeated

98   three times to ensure reproducibility. Stearic acid was applied to both ends of the samples to

99   minimize the friction between the compression anvil and the sample. The deformed samples

100 were then subjected to microstructural and textural characterization by electron backscatter

101 diffraction (EBSD) and bulk texture measurements. In order to carry out the EBSD analysis,

102 the samples were cut along the compression direction, while for the texture measurement

103 samples were cut perpendicular to the compression direction. Fig. 1 shows the schematic of

104 planes in which the EBSD and texture measurements were carried out.

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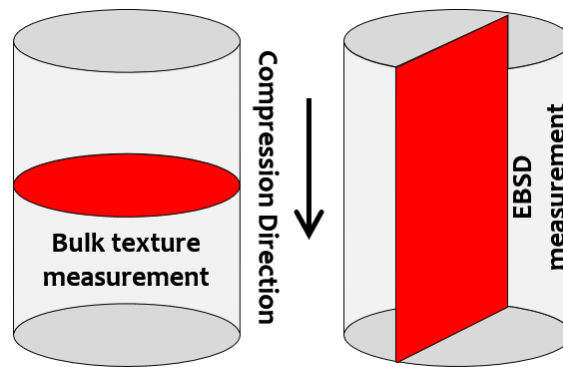
106 **Figure 1**: Schematic representing the planes for bulk texture by XRD and micro-texture by EBSD
107 measurement.
108

109 The sectioned samples were initially polished to a mirror finish using the standard silicon

110 carbide grit papers and alumina suspension. For EBSD, however, the samples were subjected

111 to polishing with 0.04 μm colloidal silica for an additional 30 minutes in order to obtain a

112 strain-free surface. EBSD measurements were performed using a scanning electron

113 microscope with a field emission gun operated (JEOL) at 20 kV voltage and 12 nA current.

114 An Oxford Nordlys detector was used to collect EBSD data with a 0.5μm step size. The

115 EBSD data were analyzed using commercially available TSL 8.0 software. Texture

116 measurements were performed using a Rigaku four circle goniometer (Ultima IV). Four

117 incomplete pole figures of tungsten b.c.c. phase namely (110), (200), (211), and (220) were

118 measured with a maximum tilt angle of 70°. The orientation distribution function (ODF) was

119   then determined from the incomplete pole figures using the M-TEX software [32]. The ODFs

120   were then used to calculate the inverse pole figures parallel to the direction of compression. It

121   should be noted that due to the lower volume fraction of the matrix, the X-ray diffraction

122   peaks associated with the f.c.c. Matrix were very weak. Therefore, the pole figure

123   measurement of the f.c.c. Phase was not carried out. The texture measurement of the f.c.c.

124   phase was done by performing large-scale EBSD maps.

125

126   **3. Viscoplastic self-consistent Simulations**

127   The viscoplastic self-consistent (VPSC) simulation predicts the texture

128   evolution and the operative deformation mechanisms for different loading conditions,

129   temperature and strain rates. Detailed information on the VPSC model can be found in the

130   manual [33]. In the following section, however, the basics of the VPSC model and the

131   simulation strategy chosen in this work are briefly explained. The grain level (ε_{ij}^g)

132   viscoplastic strain rate is related to local stress by a well-established constitutive law

133   proposed by Hutchinson [33,34].

$$\varepsilon_{ij}^g = \sum_s m_{ij}^s \gamma^s = \dot{\gamma}_0 \sum_s m_{ij}^s \left(\frac{m_{kl}^s \sigma_{kl}^s}{\tau^s} \right)^{\frac{1}{m}} \tag{1}$$

134

135   Where, $\dot{\gamma}_0$ is the reference shear rate, m is the strain rate sensitivity, τ^s is the critical

136   resolved shear stress (CRSS) of the sth slip system and m_{ij}^s is the symmetric Schmid tensor

137   which can be written as

$$m_{ij}^s = \frac{1}{2} \left(\boldsymbol{n}_i^s \boldsymbol{b}_j^s + \boldsymbol{n}_j^s \boldsymbol{b}_i^s \right) \tag{2}$$

138

139   Where, $\boldsymbol{n}$ is the slip plane normal and $\boldsymbol{b}$ is the Burgers vector. The interaction between the

140   ellipsoidal grain and HEM is defined by

6

$$\left(\varepsilon_{ij}^g - \bar{\bar{\varepsilon}}\right) = -\widetilde{M}\left(\sigma_{kl}^g - \bar{\sigma}\right) \tag{3}$$

141   Where,

$$\widetilde{M} = n^{eff}(I - s^{-1}) : S : \bar{M}^{sec} \tag{4}$$

142

143   Here, I and S represent the Identity and Eshelby tensor for a given grain. An adjustable

144   parameter n^{eff} describes the nature of linearization for the compliance of the grain-matrix

145   interactions [35]. The different values of n^{eff} implies the different nature of grain matrix

146   interaction. $n^{eff} = 0, 1, \sim20,$ and ∞ implies the Taylor, Secant, Tangent and Sachs model,

147   respectively. The vicinity effect of two phases accounts a strong correlation in morphology

148   and orientation between the grains. The 2-site self-consistent model, developed by Lebensohn

149   and Canova [36], considers the two interacting grains of different phases deforming in the

150   HEM [37]. The equations that correspond to VPSC-2S compared to the 1-site approach has

151   been tabulated by Lebensohn et. al. [38].

152   The VPSC model includes hardening via the extended Voce hardening law. This law

153   is based on the evolution of work hardening as a function of the accumulated shear strain in

154   the grain [39].

$$\tau_c^\alpha = \tau_0^\alpha + (\tau_1^\alpha + \theta_1^\alpha \Gamma)\left[1 - exp\left(-\frac{\theta_0^\alpha \Gamma}{\tau_1^\alpha}\right)\right] \tag{5}$$

155

156   Where, $\Gamma = \sum_s |\Delta\gamma^s|$ is the total cumulative shear deformation by each active system s

157   belonging to a slip mode α. τ_0^α, θ_0^α, τ_1^α, and θ_1^α are the initial CRSS, initial hardening rate,

158   back extrapolated CRSS and the asymptotic hardening rate, respectively. In the present work

159   a VPSC-2S model [36] was used, which addresses the inclusion problem for a pair of grains

160   embedded in the HEM. The two-phase model calculates one-site Eshelby tensors for the

161   individual phases as well as two-site Eshelby tensors for each phase, which act as coupling

162 factors between the eigenstrain in one inclusion and the local deviation in strain of other

163 phase [40]. Table 2 summarizes the Voce hardening parameters for a tungsten heavy alloy.

164 **Table 2** Parameters for extended Voce hardening law

Phase	Slip system family	τ_0	τ_1	θ_0	θ_1
W	$\{\bar{1}10\} < 111 >$	τ_0	235	355	0
	$\{11\bar{2}\} < 111 >$	$1.3\,\tau_0$	350	100	20
	$\{12\bar{3}\} < 111 >$	$1.5\,\tau_0$	200	100	10
Matrix	$\{111\} < \bar{1}10 >$	$0.6\,\tau_0$	200	100	0

165

166 The initial texture of the material (which is quite random, Fig. 2g) was taken as input and

167 simulations were run up to a strain of 0.69 in 69 steps. Each simulation step corresponds to a

168 strain increment of 0.01. It should be noted that the initial texture has been discretized to give

169 10,000 single orientations that will be used as input into VPSC. An aspect ratio of one was

170 used for both the phases because the microstructures for both phases showed equiaxed grains.

171 **4. Experimental Results**

172 **4.1. Initial microstructure and texture**

173   The as-sintered microstructures of the two representative tungsten heavy alloys are

174 shown in Fig. 2(a-b). The grain size of tungsten and the phase fraction of the matrix after

175 sintering are listed in Table 3. A large standard deviation in grain size was observed due to

176 the Ostwald ripening phenomenon during sintering. The phase fraction of the matrix was

177 determined using the stereological area fraction method.

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179

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180

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Table 3: Grain size and phase fraction of sintered WHA

| Sample	Grain Size of W (μm)	Phase Fraction of Matrix
80W-20M	21 ± 8	0.3
85W-15M	20.7 ± 8.4	0.23
90W-10M	22 ± 7.2	0.19
95W-5M	20.2 ± 7.3	0.13
98W-2M	20 ± 5	0.08

182

183   The alloys 80W-20M and 98W-2M were chosen because they represent the extreme

184   conditions. Both the microstructures can be characterized by the presence of coarse tungsten

185   particles surrounded by a fully wetting matrix. It can also be seen that contiguity, the W-W

186   contact fraction, and the connectivity increases with the W content. Elemental distribution

187   maps were also obtained via EDS to confirm the composition of the particles and the matrix.

188   The brighter phase consisted of pure W and the darker phase consisted of solid solution Ni-

189   24W-22Fe. The X-ray diffraction pattern shown in Fig. 2f confirms that the sample is free of

190   any strain heterogeneity or size effects, as can be seen from the relatively sharp peaks with a

191   small broadening (full width at half maximum). Aside from the peaks of the b.c.c. phase, a

192   few small peaks corresponding to the f.c.c. phase can also be observed. The presence of a

193   preferred orientation or crystallographic texture was also verified by measurement of bulk

194   texture of the initial sample. The crystal orientation or inverse pole figure map along the

195   compression direction shown in Fig. 2g suggests that the texture in the initial sample is

196   random. It should be noted that texture measurements were undertaken for all five samples.

197   However, for brevity, the IPF‖CD of only 80W-20M is shown. It was also observed that the

198   texture of the other compositions was random.
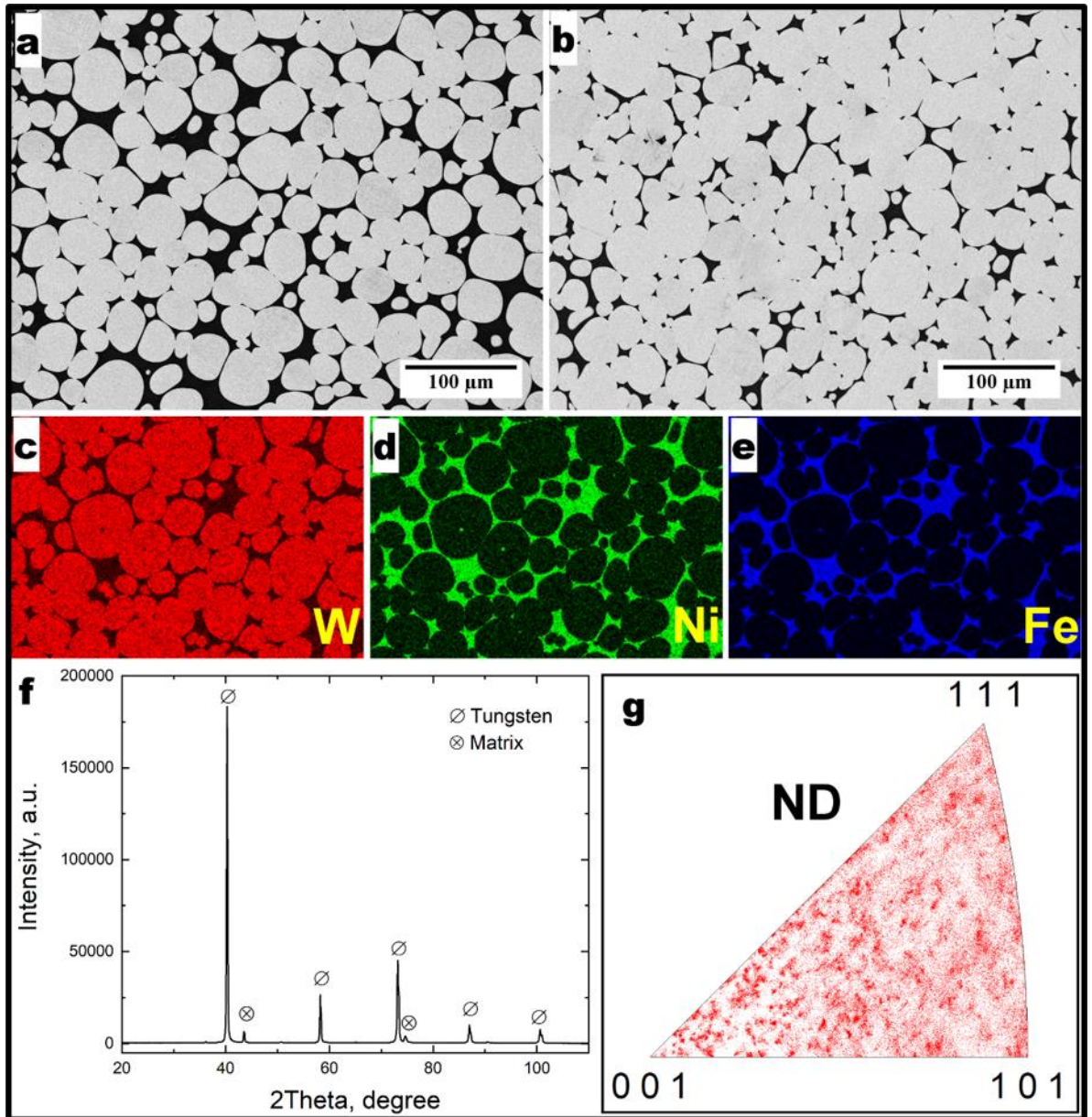
Figure 2:(a) Backscattered electron images for 80W-20M alloy (b) Backscattered electron images for 98W-2M alloy (c-e) elemental distribution maps by EDS (f) x-ray diffractogram for 80W-20M alloy (g) Inverse pole figure plotted parallel to the compression direction for 80W-20M alloy

208   **4.2. Texture evolution of tungsten heavy alloy during uniaxial compression**

209   Figure 3 shows the true stress - true strain curve and work hardening rate $\left(\frac{d\sigma}{d\varepsilon}\right)$ vs

210    $\sigma - \sigma_0$ for all the alloys. All the sample behaved in similar manner and the dominance of the

211   stage III deformation [41] was evident as a straight line in work hardening curve.

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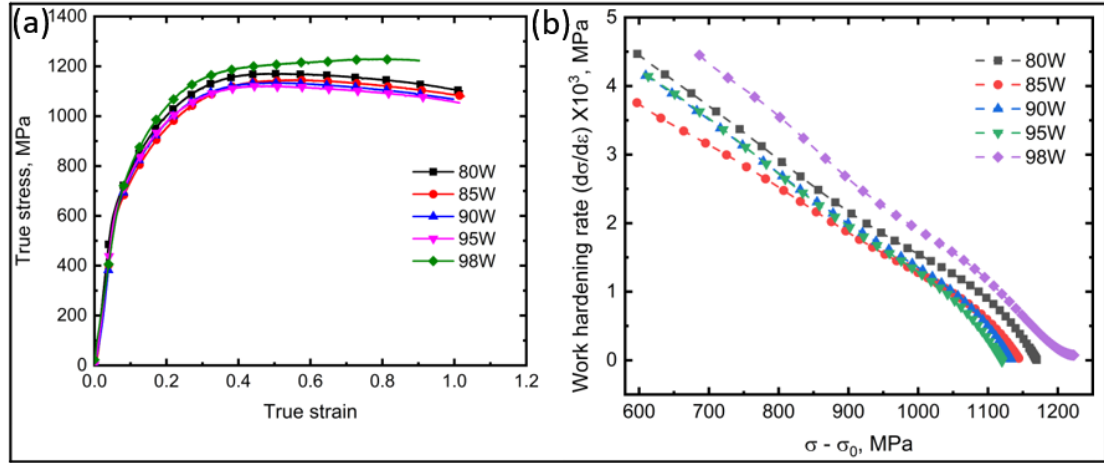
213   **Figure 3**:(a) True stress-true strain plot of WHAs (b) Work hardening rate vs $\sigma - \sigma_0$ of
214   WHAs

215   Figure 4a shows the IPF‖CD (compression direction) for all the five alloy compositions

216   considered in the present work. As can be observed, the classical double-fiber texture with

217   weak <100> fiber and major <111>‖CD fiber is obtained after uniaxial compression. This is

218   the typical texture found in many b.c.c. metals and alloys after uniaxial compression.

219   However, a closer look at the IPF's suggests that there is a systematic influence of the

220   composition on the texture evolution, mainly with regard to the relative proportion of <100>

221   and <111> fibers. This behavior is elegantly shown in Fig. 4d where the ratio of the volume

222   fraction of <100> and <111> fibers is plotted. It can be clearly seen that the volume fraction

223   ratio increases with increasing tungsten content. The volume fraction of the individual fibers

224   is also shown in Fig. 4c. Although the <111> fiber is the strongest for all of the present

225   compositions, it is apparent that the volume fraction of <100> fiber increases steadily with an

226   increase in the tungsten content. As already mentioned, texture measurements via XRD were

11

227 not possible for the f.c.c phase because of very weak peaks (Fig. 2f). Therefore, the texture

228 measurement of the matrix phase was carried out via EBSD. Fig. 4b shows inverse pole

229 figure for the f.c.c. phase in the compression direction. It can be seen that the classical

230 <110>∥CD texture evolves after uniaxial compression up to a height reduction of 50%. The

231 texture of the f.c.c. phase is quite weak (2.5 mrd) compared to the main tungsten phase (8.0

232 mrd). This weak texture can be attributed to the relatively lower volume fraction of the f.c.c.

233 phase compared to the b.c.c. phase. Therefore, in the following we will concentrate entirely

234 on the texture development of the b.c.c. tungsten phase, with reference to the f.c.c. matrix

235 phase wherever this is required.

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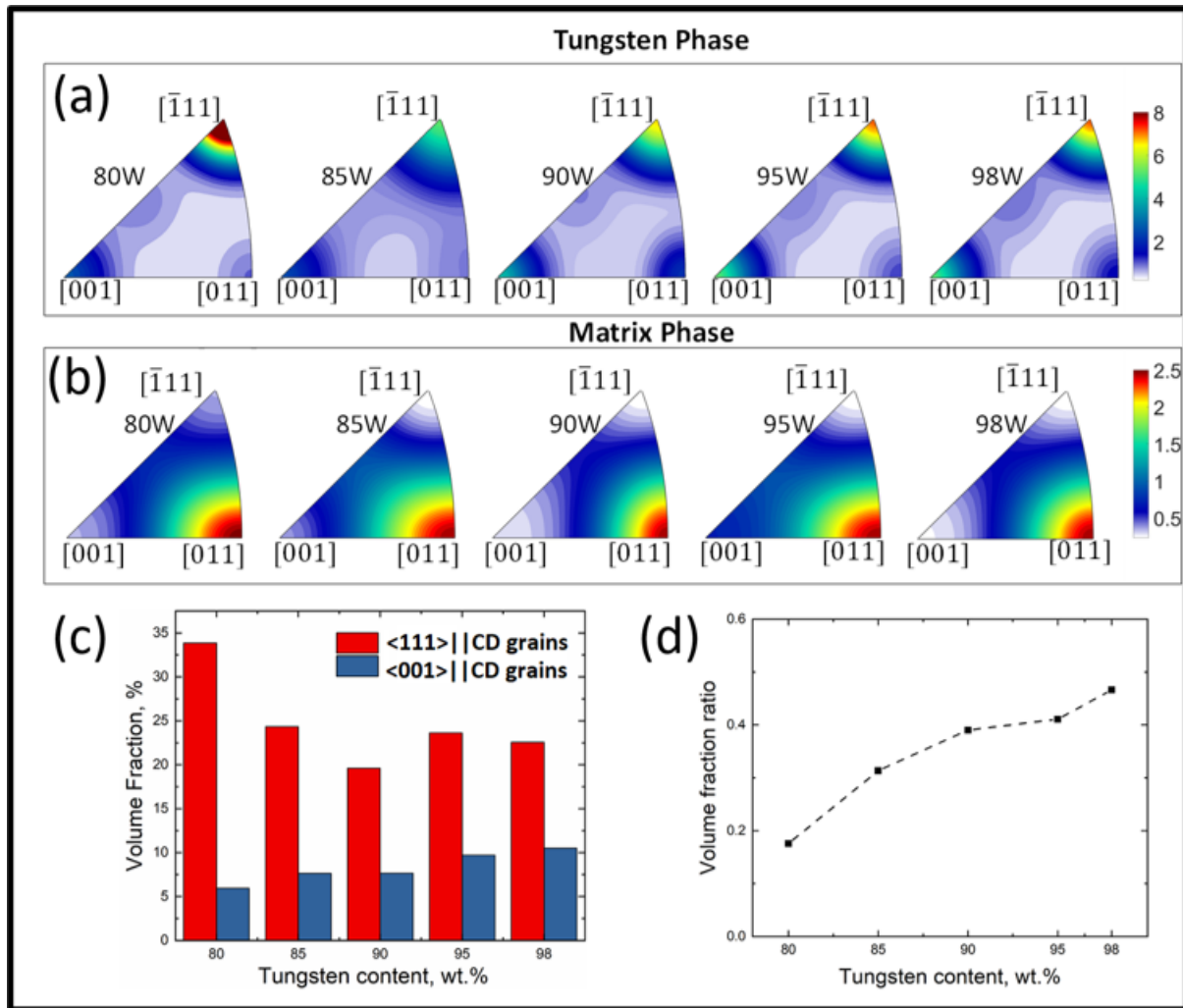
237 **Figure 4**:(a-b) Inverse pole figures plotted parallel to compression direction for different
238 composition of tungsten and matrix (c) volume fractions of <111> and <100> fibre for

239 different composition (d) volume fraction ratio of <100> to <111> fibre as a function of
240 tungsten content.

4.3. Microstructural evolution during uniaxial compression of tungsten heavy alloy

242 The inverse pole figure maps and phase maps of the deformed tungsten heavy alloys are

243 shown in Fig. 5a and 5b, respectively. The color code to represent the grain orientations is

244 shown in Fig. 5e. The compression direction (CD) is marked in the IPF maps. The maps

245 clearly show the orientation gradient in the microstructure, which means a heterogeneous

246 deformation.
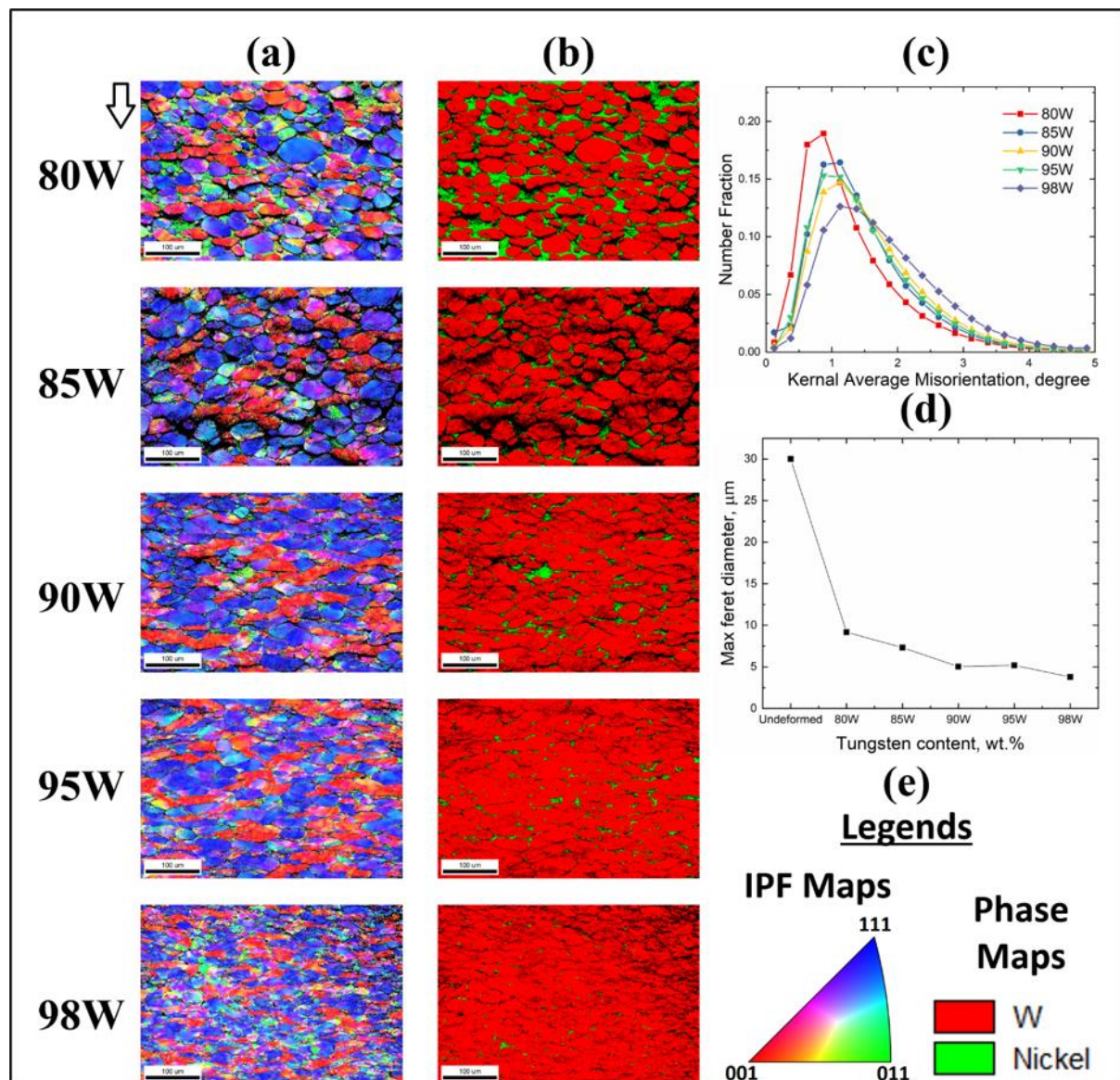
Figure 5: (a-b) Inverse pole figure maps plotted parallel to compression direction and phase maps for different compositions, respectively. (c) Kernel average misorientation distribution profiles. (d) Feret diameter as a function of tungsten content. (e) IPF color key.

The presence of an intragranular orientation gradient is common in deformed microstructures and depends on the initial orientation as well as neighboring grains. In addition, deformation banding can be observed in the microstructures which can lead to fragmentation of grains. Apart from these general characteristics, there is also a systematic influence of the composition on the development of the microstructure. As can be observed, the extent of the strain heterogeneity of the tungsten phase increases with increasing tungsten content. This heterogeneity can be attributed to the strain partitioning effect between the soft matrix phase and the hard tungsten phase. With an 80W-20M alloy, the matrix can accommodate a significant amount of imposed deformation compared to the 98W-2M alloy, where the matrix volume fraction is minimal. With the 98W-2M alloy, the tungsten phase must accommodate most of the deformation imposed. This is elegantly captured by the aspect ratio of the tungsten particles, where the particles in the 80W-20M alloy are relatively equiaxed compared to 98W-2M alloy, where the particles have developed a pancake shape and are elongated in the radial direction. The Kernel Average Misorientation (KAM) plot (Fig. 5c) also confirms this observation. The KAM represents the average misorientation of a pixel with its neighboring pixels and is therefore ideally suited for estimating the strain heterogeneity. Fig. 5c indicates that the KAM distribution of tungsten particles shifts to higher angles with increasing tungsten content. This confirms our argument that the dislocation activity and strain heterogeneity of the tungsten particles is a strong function of the matrix content. Additional evidence of this behavior is obtained from the Feret diameter of the particles. The Feret diameter corresponds to the greatest distance between the two parallel lines on the opposite side of randomly oriented particles. Therefore, a reduction in the

14

274 Feret diameter is an indication of a reduction in grain size and grain fragmentation of

275 tungsten particles. As can be seen in Fig. 5d, the Feret diameter is the smallest for the 98W-

276 2M alloy. After analyzing the phase-dependent deformation, we now shift our attention to the

277 orientation-dependent deformation of tungsten particles. The tungsten particles constitute the

278 major portion of these alloys and therefore require further investigation of their deformation

279 behavior. In this regard, the two orientations correspond to the major texture components i.e.,

280 <100> and <111>∥CD were partitioned with a tolerance angle of 10°.
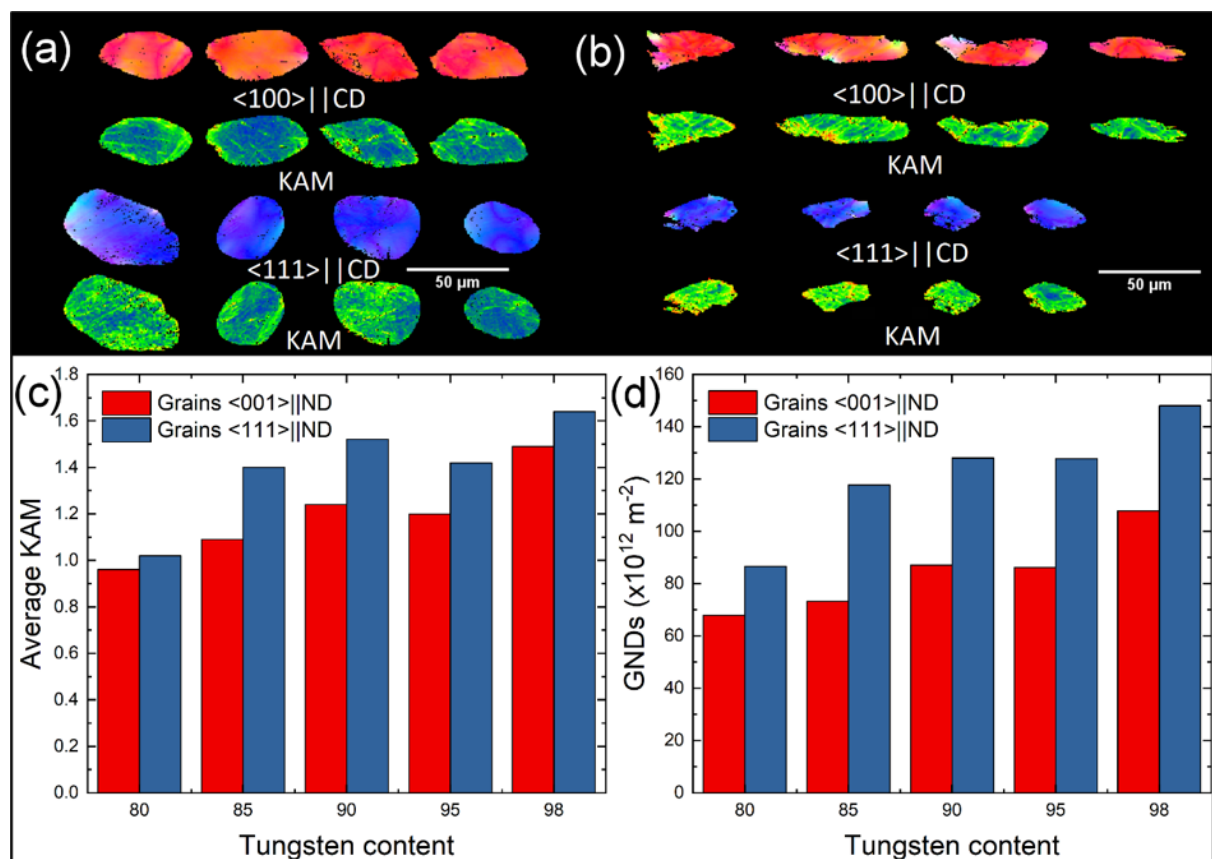
282 **Figure 6**: (a-b) Set of grains representing <111> and <100> fibers with their KAM map for
283 80W-20M and 98W-2M, respectively. (c-d) KAM and GND histogram as the function of
284 tungsten content.

285

286 Figure 6(a-b) highlights some representative grains of the <100> and <111> orientations. As

287 before with the strain partitioning between the phases, we call up the KAM again to analyze

288   the deformation behavior of <100> and <111> oriented grains. As can be observed in Figure

289   6c, the average KAM for <111> oriented grains compared <100> oriented grains is higher

290   regardless of the alloy composition. However, the difference between the KAM values

291   increases as the tungsten content increases. This can be explained by the higher strain

292   accommodation of tungsten particles with increasing tungsten content. A simplified

293   explanation of the higher KAM value of <111> oriented grains compared to <100> oriented

294   grains can be provided with regard to the Taylor factor. As calculated for axisymmetric

295   deformation, the Taylor factor is 3.67 for <111> oriented grains compared to 2.44 for <100>

296   oriented grains. Therefore, more work or plastic shearing is required in the <111> grains in

297   order to achieve the same equivalent strain compared to <100> grains. This also increases the

298   dislocation activity in <111> grains higher compared to <100> grains on the microscopic

299   length scale, which leads to the formation of dislocation boundaries, which in turn lead to a

300   higher KAM. The geometrically necessary dislocation density (Fig. 6d) for the two grain

301   families also confirms our arguments.

302   **5. Simulation results**

303   As mentioned earlier, VPSC was used to perform texture simulations. It is known that the

304   texture evolution in b.c.c. metals and alloys can be attributed to pencil glide on {110}, {112}

305   and {123} slip planes with the common <111> slip direction [42]. Therefore, we also selected

306   pencil glide in VPSC for performing texture simulations. Based on a comparison between

307   experimental and simulated texture, it was found that another important aspect to decide

308   before executing the VPSC code is the deformation mode. The VPSC code allows the n^{eff}

309   parameter to be tuned to mimic the two extremes of plastic deformation viz. the upper bound

310   Taylor type and the lower bound Sachs type. As can be seen from equation 6, $n^{eff} = 0$

311   corresponds to a Taylor type deformation, while ∞ corresponds to Sachs type deformation.

312   Since the mode of deformation is unknown in advance, we performed texture simulations

313 taking into account the different modes and based on the agreement between experimental

314 and simulation results, the mode of deformation is determined. It should be noted that

315 n^{eff}=100 is enough to simulate the Sachs-type deformation behavior as it is physically

316 impossible to use infinity in the VPSC code. Other key parameters required to run the VPSC

317 simulations such as the velocity gradient, total strain imposed, and strain increment are

318 specified in section 3. It has been observed that secant type deformation with simultaneous

319 rotation of adjacent grains adequately reproduces the experimental results. This can be

320 justified physically with the requirement of strain compatibility at the tungsten-tungsten and

321 tungsten-matrix interface and the equiaxed nature of the tungsten particles. It is also generally

322 accepted that strain compatibility is a more important criterion than stress compatibility

323 (Sachs mode) during plastic deformation. In Fig. 2(a-b), it can be observed that the contact

324 between tungsten-tungsten particles is much more prevalent in the 98W alloy than in 80W

325 alloy. It is known that neighboring orientations can significantly change the local velocity

326 gradient compared to the macroscopically imposed velocity gradient, which in turn can lead

327 to completely different rotation paths and thus final texture [43]. In the VPSC model, the

328 influence of neighbors can be taken into account in an empirical way by randomly pairing the

329 grains, which are then caused to co-rotate. The co-rotation scheme was used in the VPSC 7D

330 model by Tomé et al. [44]. This scheme leads to a different rotation path for similarly oriented

331 grains based on the chosen neighbor. As can be seen from Fig. 2(a-b), a single tungsten

332 particle is in contact with an average of five other particles for the 98W alloy compared to

333 two for the 80W alloy. Therefore, random pairs of five and two particles were considered for

334 performing texture simulations of 98W and 80W alloy, respectively.
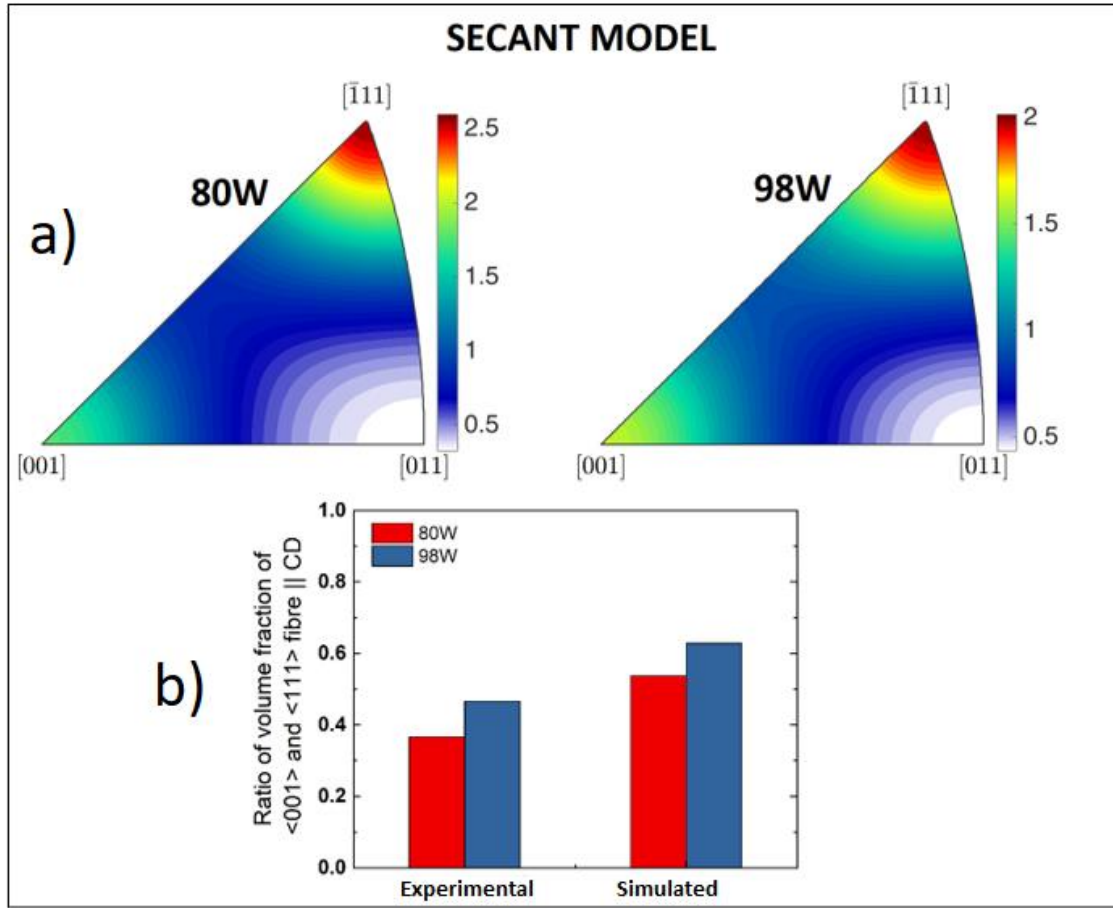
Figure 7: (a) Predicted inverse pole figure (IPF) parallel to compression direction by Secant model for the two extreme compositions considering the connectivity of the tungsten particles. (b) Comparison between experimental and simulated ratios of volume fraction of <100> and <111> fibres.

Fig. 7 shows the simulated inverse pole figures together with the comparison between the experimental and the simulated volume fraction ratio. It can be said that the agreement between experimental and simulation results matches significantly in agreement when the grains are paired and rotated together. The intensity near the <100> corner is clearly high for the 98W-2M alloy compared to the 80W-20M alloy. The simulated volume fraction ratio of the two alloys also follows a trend similar to that observed experimentally. Although this is a simplified way of looking at the effect of neighboring particles, it underlines their role in plastic deformation and the resulting texture development. It should be noted that all of these

349 VPSC simulations were performed with considering the two-phase scenario i.e., VPSC-2S

350 model. The phase fraction was suitably set in VPSC depending upon the alloy composition.

351 Thus, in addition to the texture of the tungsten particles, the simulated texture of the matrix

352 was also obtained. Fig. 8(a-b) shows the inverse pole figure in the compression direction, the

353 classic <110> fiber texture during f.c.c compression is satisfactorily reproduced by VPSC

354 simulations. The activity diagrams showing the strain partitioning and the average active

355 systems per grain (AVACS) between the two phases are shown in Figure 8b.

356
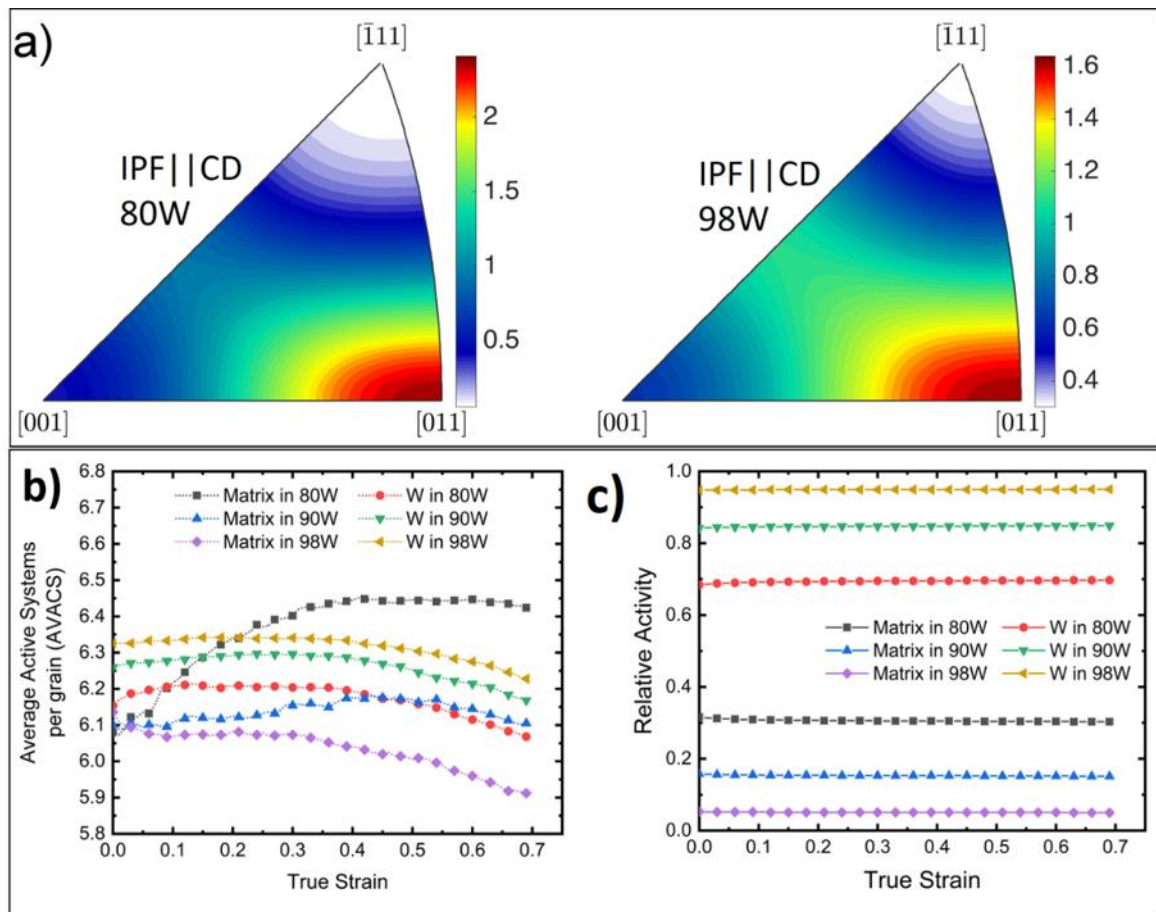
357 **Figure 8**: (a) Inverse pole figure (IPF) parallel to compression direction predicted by Secant
358 model for matrix for the two-extreme composition. (b) Strain partitioning represented by the
359 relative activity of the slip systems as a function of true strain. (c) Predicted average active
360 slip systems per grain as a function of true strain.

361

362 On average, six slip systems were active and showed a deformation close to the upper bound

363 model in all the alloy. The tungsten particles, which are the dominant phase, bear most of the

364 externally imposed deformation compared to the matrix phase, so that the relative activity

365 (shown in Fig. 8c) of tungsten is always higher than that of the matrix.

366 **6. Discussion**

367 The texture evolution during compression can be fully understood by showing the lattice

368 rotation behavior in an inverse pole figure. A schematic representation of the lattice rotation

369 is shown in Fig. 9a.

370
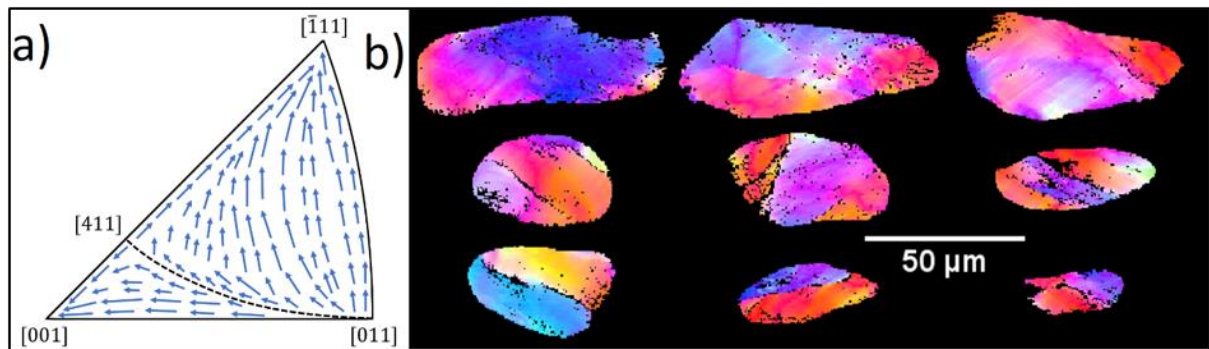
371 **Figure 9:** (a) Schematic of lattice rotation during uniaxial compression for b.c.c. (b)
372 Representative grains showing the orientations lying on both side of divergent line in a single
373 grain.

374

375 The lattice rotation path was obtained by Rosenberg and Piehler [45] by implementing the

376 pencil-glide hypothesis. As can be seen, the grains tend to rotate in direction <111> or <100>

377 depending upon the orientation of the compression axis. All the grains lying above the [110]-

378 [411] line would rotate towards <111>, whereas the grains lying below the [110] - [411] line

379 would rotate in the direction of <100>. The [110] - [411] line is generally known in the

380 literature as 'divergent line' [46]. For an initial random texture, a majority of the grains would

381 be lying above the divergent line compared to the one below. As a result, a large proportion

382 of the grains would come close to <111> compared to <100>. Rosenberg and Piehler [47]

383   calculated using simulations that for an initial random texture 74% of the grains would rotate

384   in the direction of <111>, compared with 26% in the direction <100>. This explains the

385   experimental observation of the relative dominance of <111> fibers compared to <100>

386   fibers, regardless of alloy composition. It should be noted that the above rotational paths were

387   predicted without considering the influence of neighboring grains. As has been discussed by

388   several researchers in the past, the deformation behavior of individual grains depends heavily

389   on their neighborhood. The local state of stress within the individual grains can, depending on

390   the environment, deviate significantly from the macroscopic imposed deformation, which in

391   turn influences the selection of active slip systems and thus the lattice reorientation.

392   However, the determination of the local stress state is not easy and requires high precision

393   measurements of the elastic strains in relation to internal stresses using high-resolution EBSD

394   [48]. Otherwise, three-dimensional in-situ diffraction experiments with high-energy X-rays and

395   neutrons that can penetrate deep into the crystals are required to measure the full elastic strain

396   tensor for several individual grains. Even with such high-end experiments, the best approach

397   to determining the exact state of stress is still being discussed in the literature. Therefore, we

398   will only make a qualitative attempt to understand the role of the local neighborhood in the

399   texture evolution. In the present work the effect of the local neighborhood manifests itself in

400   the form of an increasing volume fraction ratio of <100> and <111> fibers with increasing

401   tungsten content. As previously demonstrated via VPSC, running Secant simulations without

402   considering the neighboring orientations did not provide a satisfactory match to the

403   experimental texture, particularly for the 98W-2M alloy. Only when texture simulations were

404   performed by pairing five randomly oriented grains, a reasonable match was reached. A clear

405   picture of the role of the neighbors can be obtained from the lattice rotation schematic in Fig.

406   9a. It can be considered that the orientations that are close to the deviation line follow rather

407   unpredictable rotation paths compared to orientations that are far away from the deviation

408   line. A slight fluctuation due to the local neighborhood can lead to the orientation being

409   shifted from above the divergence line downwards and vice-versa. As a result, the grain will

410   now follow completely new rotation path compared to the path it should take based on its

411   initial orientation. On the other hand, the grains that are far from the divergent line can pick

412   up small random fluctuations due to the neighbors and continue to follow the predicted path

413   of rotation, albeit at reduced speeds. Looking at the initial random texture in the present case,

414   where a large proportion of grains lie above the divergent line, it can be said that a greater

415   number of grains make the transition from above the divergent line to the bottom and not vice

416   versa. Subsequently, these grains then rotate in direction <100> compared to <111>. The

417   rotation in the <100> direction is also energetically favourable since the Taylor factor is

418   steadily decreasing [49]. It is known that grains with a lower Taylor factor are considered to be

419   'soft grains' in which the imposed deformation can be easily accommodated, compared to

420   'hard grains' with a higher Taylor factor. The hard grains develop more deformation

421   heterogeneities compared to the soft grains and are therefore more sensitive to the local

422   neighborhood. For a 98W-2M alloy, where contact between tungsten-tungsten particles is

423   significant, the fluctuations are more frequent than for an 80W-20M alloy, where the contact

424   between tungsten-tungsten particles is limited. As a result, the 80W-20M alloy will follows

425   the predicted lattice rotation paths and develops a significantly stronger <111> fiber

426   compared to the <100> fiber. On the other hand, the 98W-2M alloy develops a stronger

427   <100> fiber with high probability of fluctuations. Further confirmation of our arguments can

428   be obtained from EBSD measurements. As previously shown, the deformation heterogeneity

429   is significantly higher for the 98W-2M alloy compared to the 80W-20M alloy. The amount of

430   grain fragmentation, shown in terms of Feret diameter, is also higher for the 98W-2M alloy.

431   All of these effects can be attributed to unforeseen rotation paths in the 98W-2M alloy due to

432   the local neighborhood, which prevents homogenous deformation of the grain as a whole.

433 Different parts of the same grain deform via different slip systems, which leads to the

434 development of a strong orientation gradient and ultimately to fragmentation. Some

435 representative grains are shown in Fig. 9b where it can be observed that one part of the grain

436 is above the divergence line while the other is below it. This supports our argument that a

437 higher probability of fluctuations could be the determining factor for a stronger <100> fiber

438 in the 98W-2M alloy. Other theories of texture evolution such as the changing the mode of

439 deformation from Taylor-type to Sachs-type to explain the strengthening of <100> fiber is

440 not applicable since Sachs deformation results in an inappropriately strong <100> fiber, this

441 is not observed experimentally. The overall texture is still dominated by <111> fibers,

442 although the random fluctuations slightly increase the volume fraction of <100> fibers. Also,

443 the role of strain rate sensitivity, which is sometimes used in the texture community, is

444 limited here because the deformation was performed at room temperature and at nominal

445 strain rates. Therefore, it can be said that the shift in orientations along the divergent line due

446 to local neighborhood provides a reasonable explanation for the texture evolution of b.c.c.

447 tungsten particles. The texture evolution of the matrix phase can again be understood by the

448 schematic shown in Fig. 9a. Since the slip systems in f.c.c. have their plains and directions

449 interchanged with respect to b.c.c., one can say that the direction of rotation is opposite to

450 that shown in the schematic diagram. In this case, the grains aggregate in the vicinity of

451 <110> and the divergent line behaves like a convergent line. Since the grains tend to rotate in

452 direction <110> regardless of their initial orientation, the role of local neighborhood or

453 random fluctuations during f.c.c compression is limited.

454 **7 Summary**

455 In the present work a uniaxial compression test was carried out in order to understand the

456 deformation mechanisms and the texture evolution of tungsten heavy alloys. The most

457 important findings of the present work are summarized below.

458   1. The texture evolution of the b.c.c. tungsten particles can be characterized by the

459   development of <111> + <100> double fiber texture, whereas a <110> fiber evolved

460   in the f.c.c. matrix phase. The effect of composition is manifested in terms of relative

461   proportion of <100> and <111> fibers where the volume fraction ratio of <100> and

462   <111> fibers increase with increasing tungsten content.

463   2. Texture simulations via VPSC suggested that a secant type deformation pattern was

464   followed in the WHA instead of the Sachs-type deformation. However, Secant-type

465   deformation combined with the lattice corotation scheme to include the effect of

466   neighboring orientations was essential to correctly reproduce the experimental

467   textures. A five-grain pair was used for the 98W-2M alloy, while a two-grain pair was

468   used for the 80W-20M alloy to run the simulations.

469   3. The physical interpretation of the role of neighbors in increasing the <100> fiber is

470   provided in view of a high probability of fluctuations in the 98W-2M alloy leading to

471   a shift in orientations from above the [110]-[411] divergent line to below it and the

472   subsequent rotation in the direction of the <100> corner.

473

477 **Conflict of Interest**

478 The authors have not conflict of interest to declare.

479 **Data Availability statement**

480 Data will be made available on request

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481

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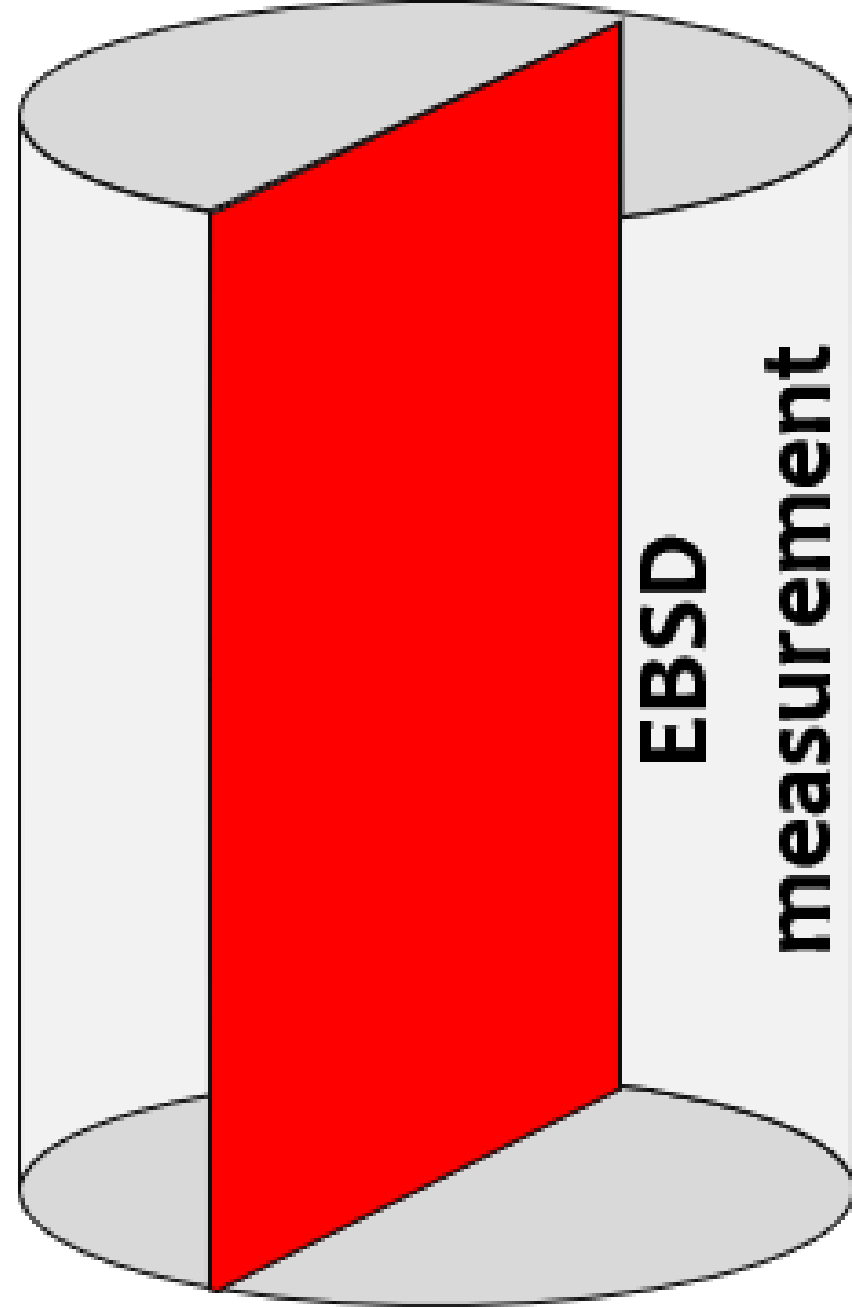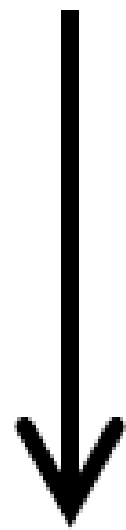568   *Engineering*, vol. 304, 2018, p. 12003.
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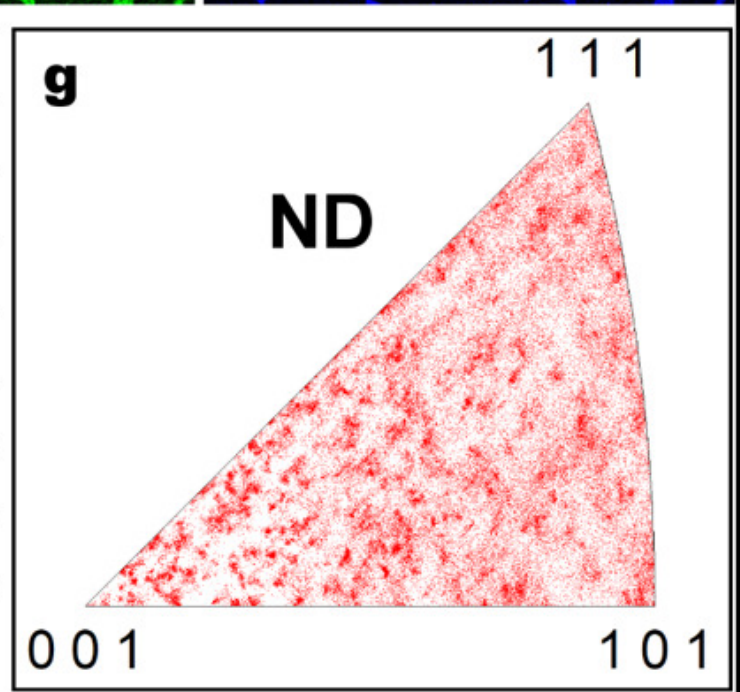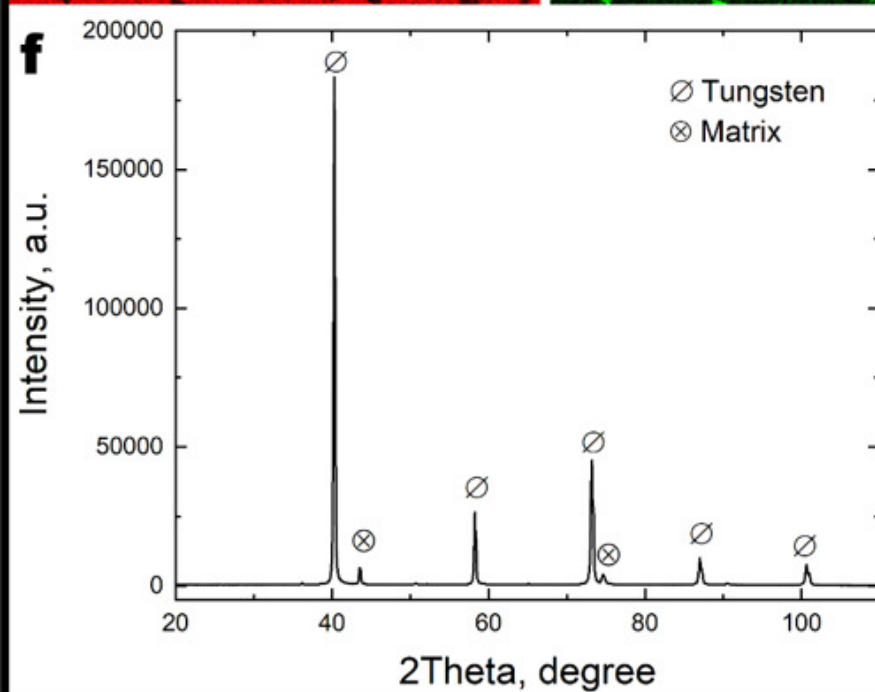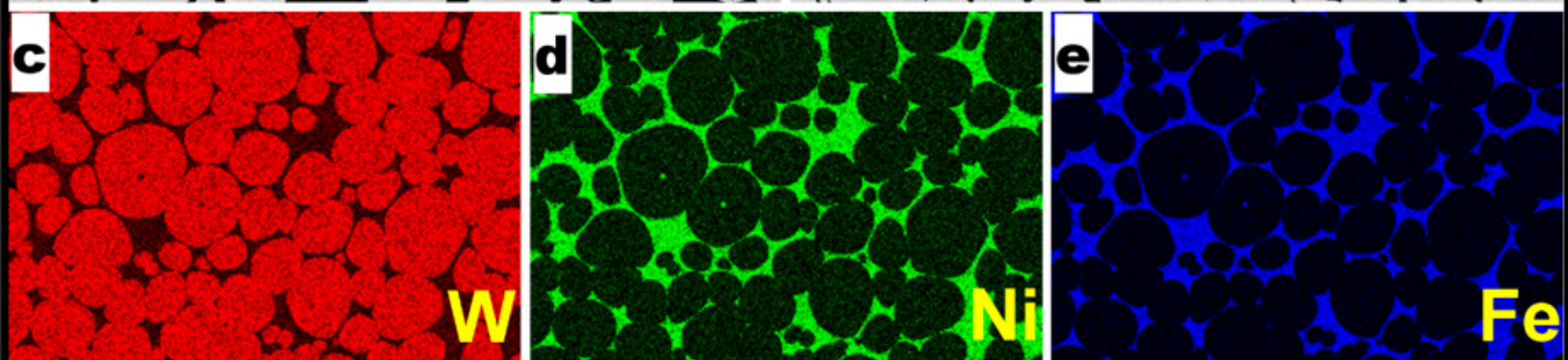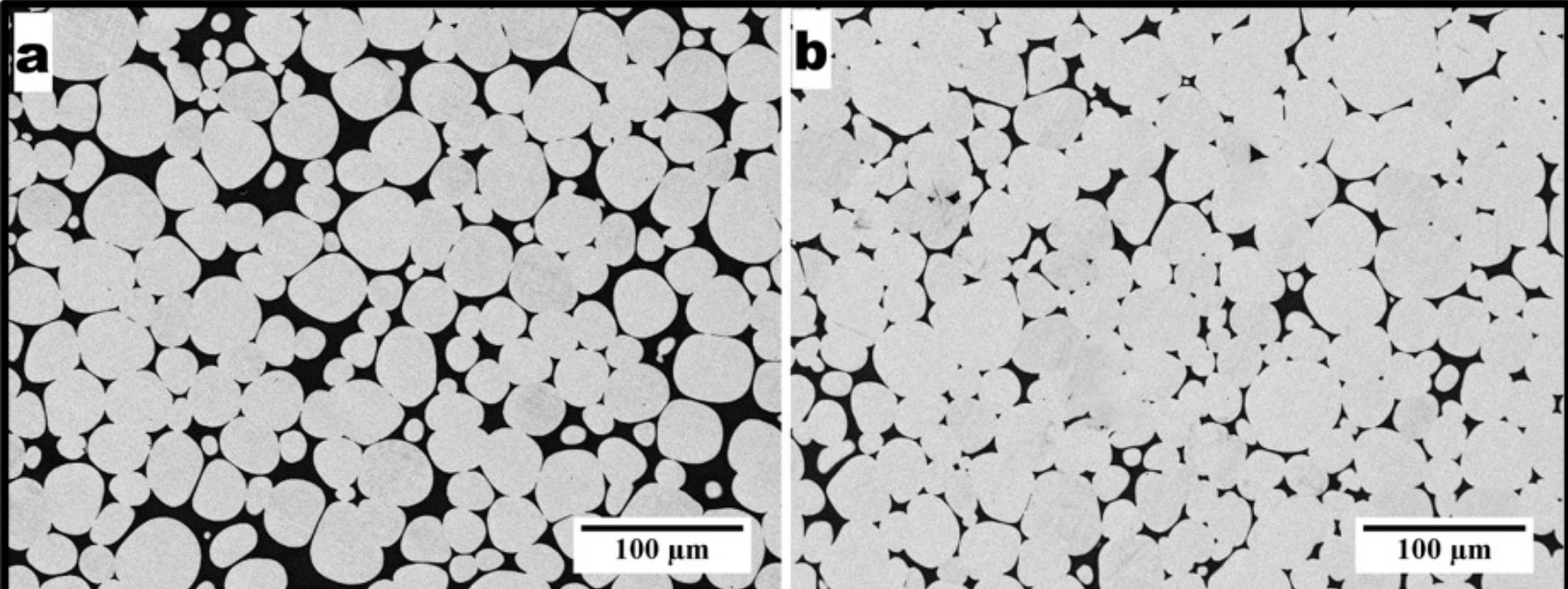570   1705–12.
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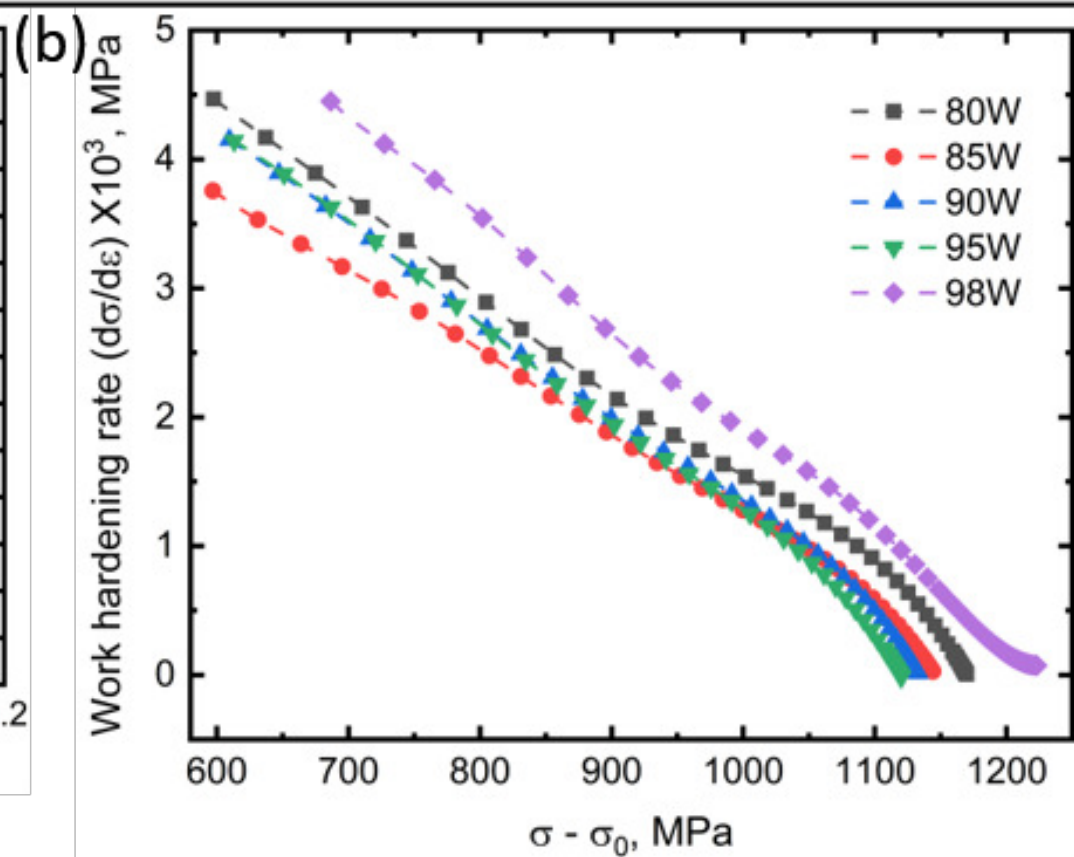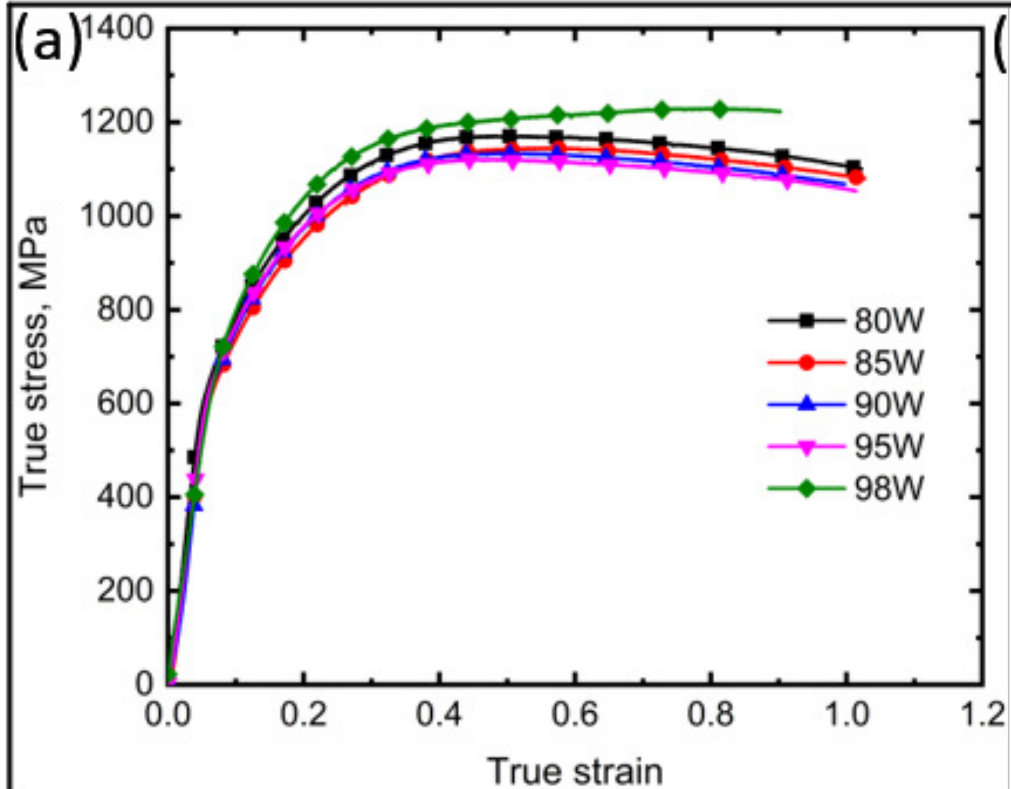572   *Magazine and Journal of Science*, 1951, vol. 42, pp. 616–35.
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Bulk texture measurement
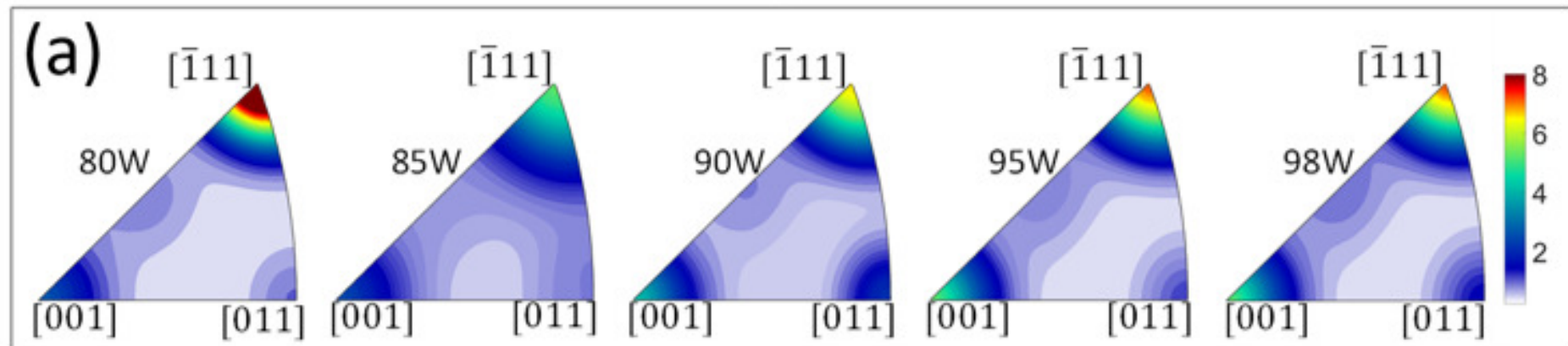
Compression Direction

EBSD measurement

f

Intensity, a.u.

⊘ Tungsten
⊗ Matrix

2Theta, degree

g

1 1 1

ND

0 0 1   1 0 1

(a) True stress–true strain curves and (b) work hardening rate $(d\sigma/d\varepsilon) \times 10^3$ versus $\sigma - \sigma_0$ for 80W, 85W, 90W, 95W, and 98W.

Tungsten Phase

(a)

[$\bar{1}$11] 80W [001] [011]
[$\bar{1}$11] 85W [001] [011]
[$\bar{1}$11] 90W [001] [011]
[$\bar{1}$11] 95W [001] [011]
[$\bar{1}$11] 98W [001] [011]

Matrix Phase

(b)

[$\bar{1}$11] 80W [001] [011]
[$\bar{1}$11] 85W [001] [011]
[$\bar{1}$11] 90W [001] [011]
[$\bar{1}$11] 95W [001] [011]
[$\bar{1}$11] 98W [001] [011]

(c)

<111>||CD grains
<001>||CD grains

Volume Fraction, %

Tungsten content, wt.%

(d)

Volume fraction ratio

Tungsten content, wt.%

(a)

(b)

(c)

(d)

(e)

80W

85W

90W

95W

98W

Legends

IPF Maps

Phase Maps
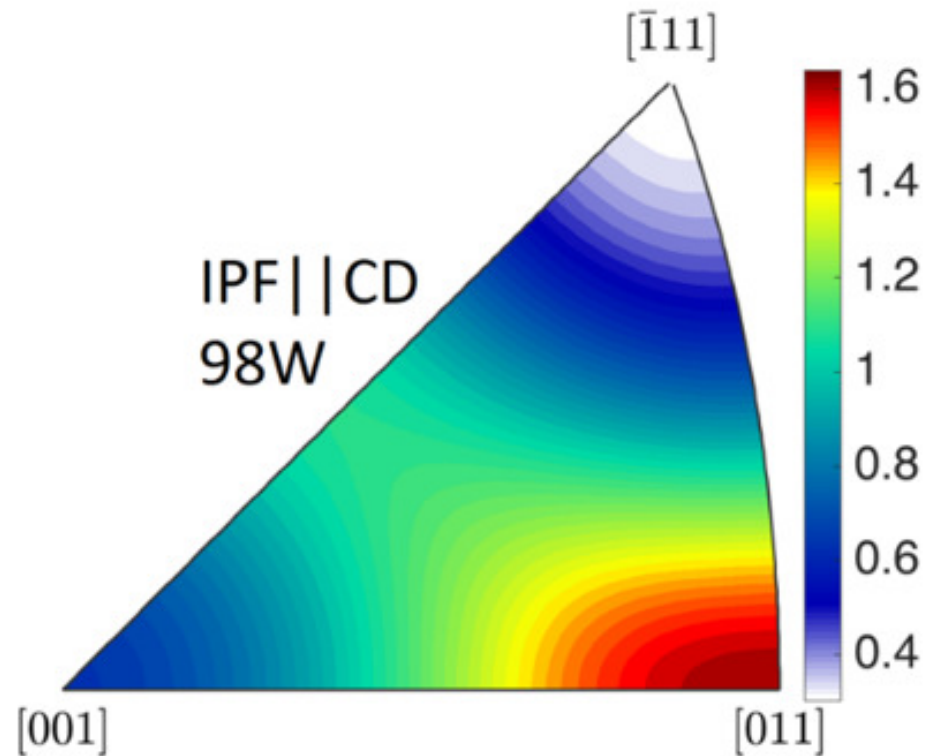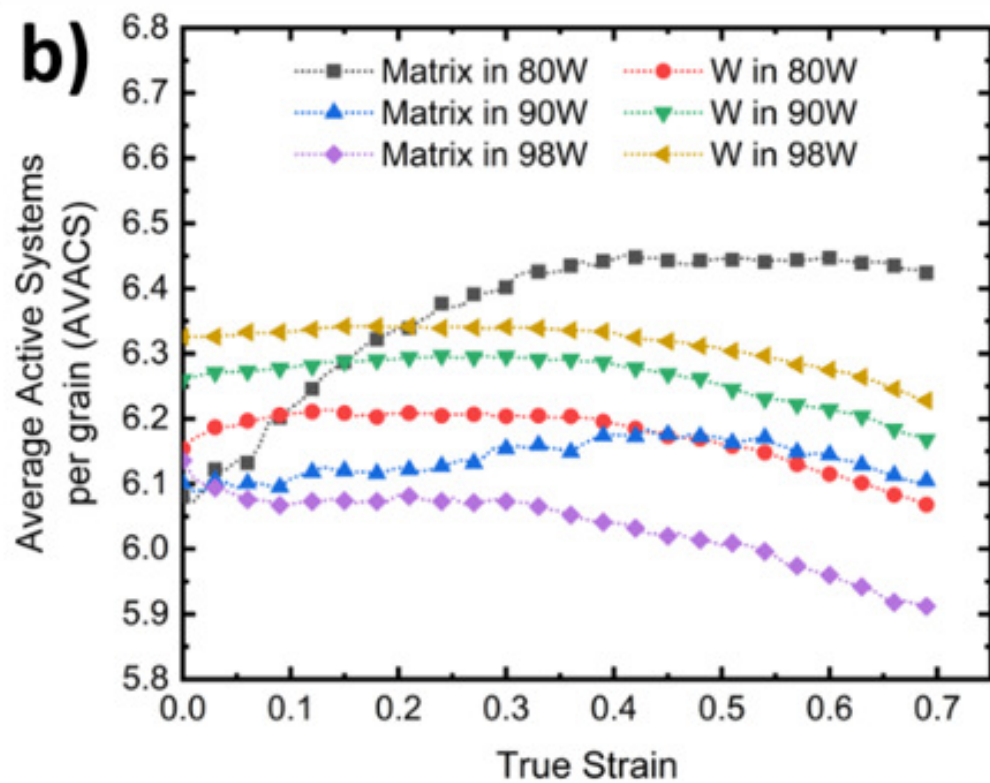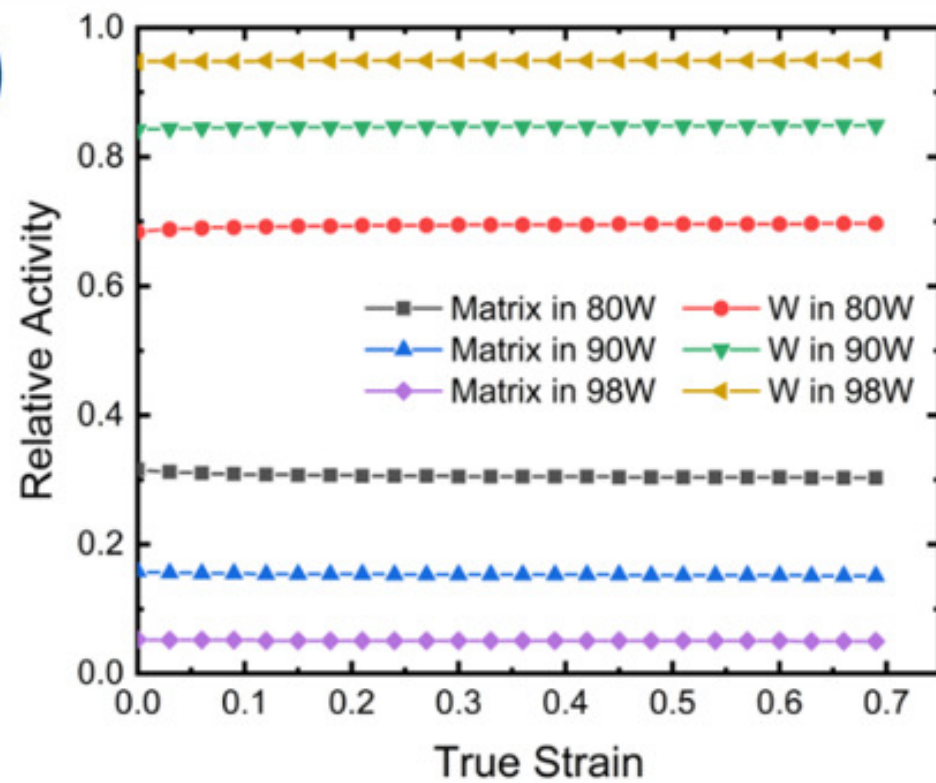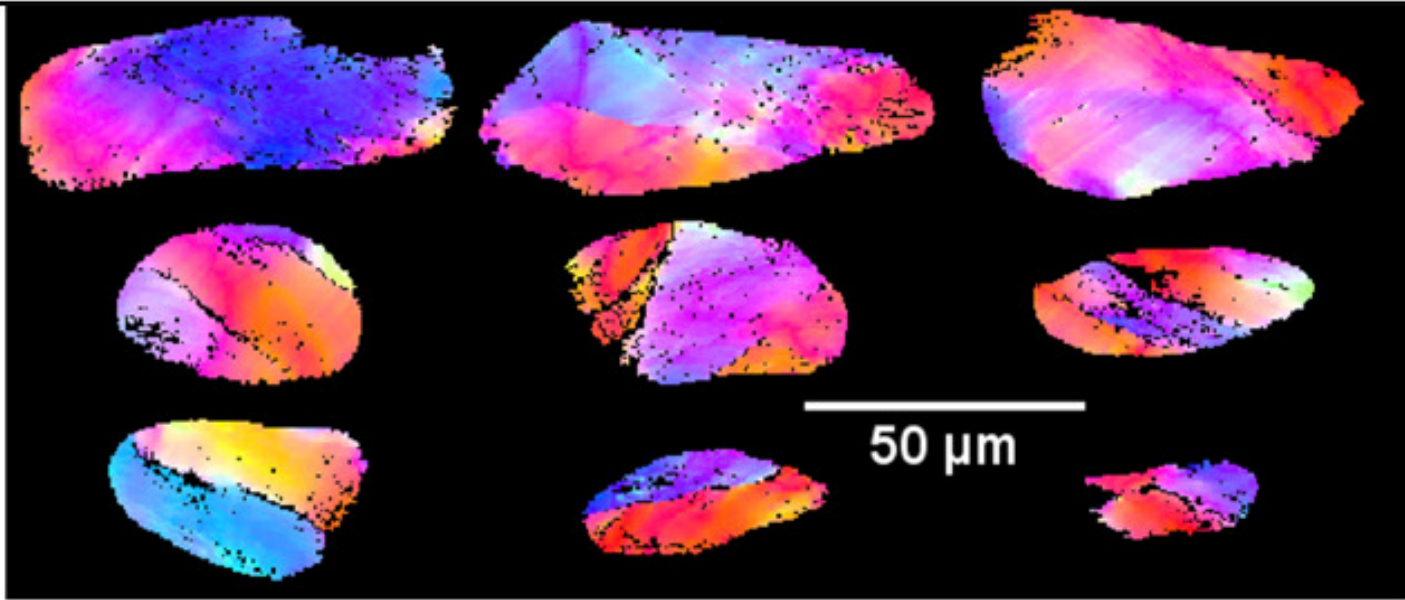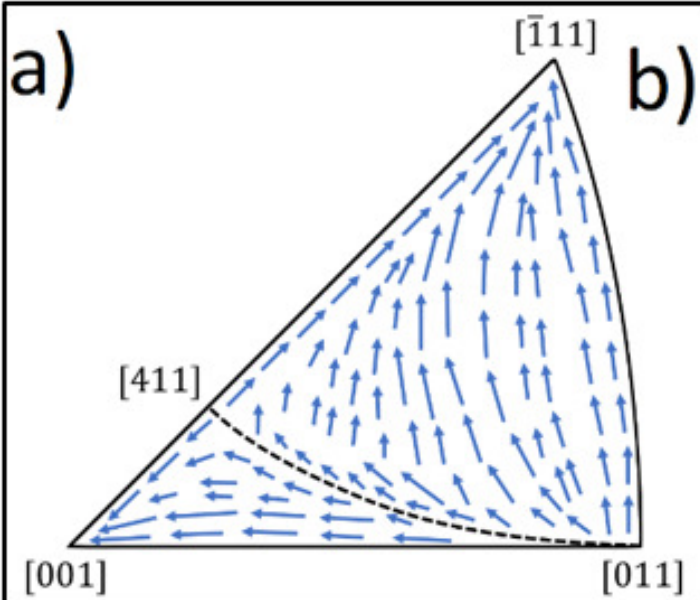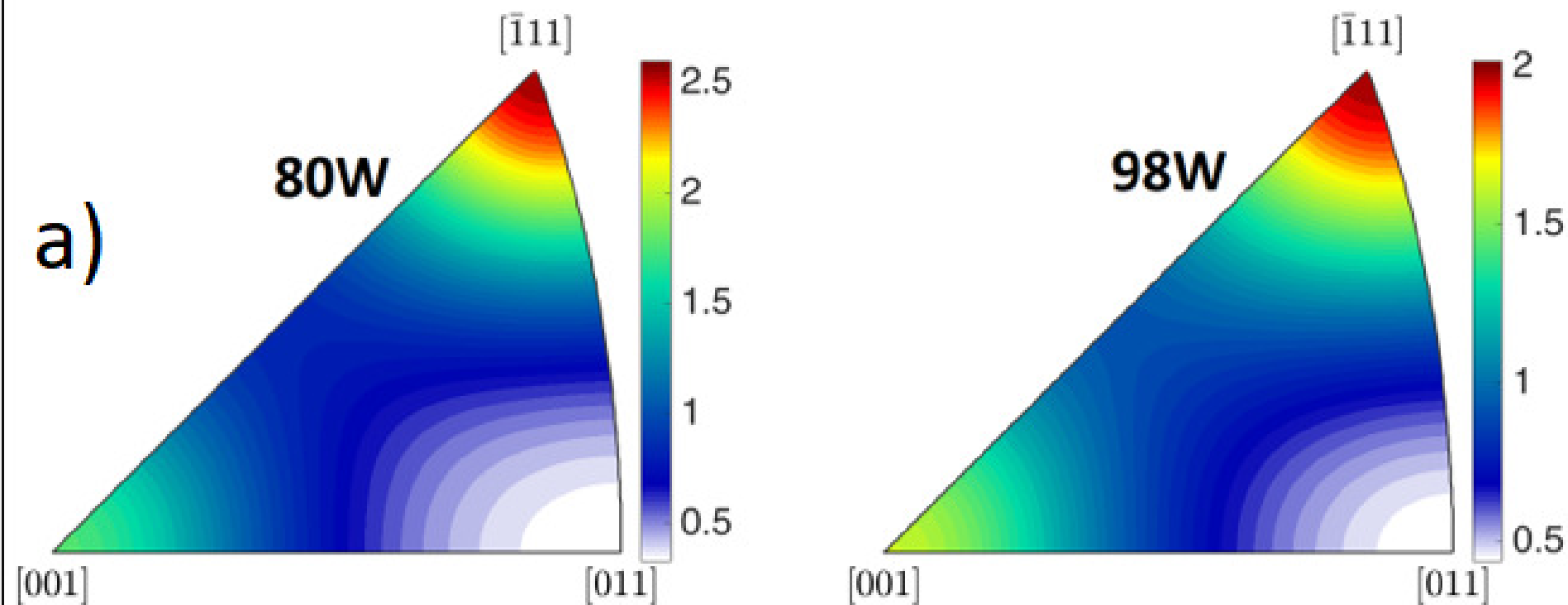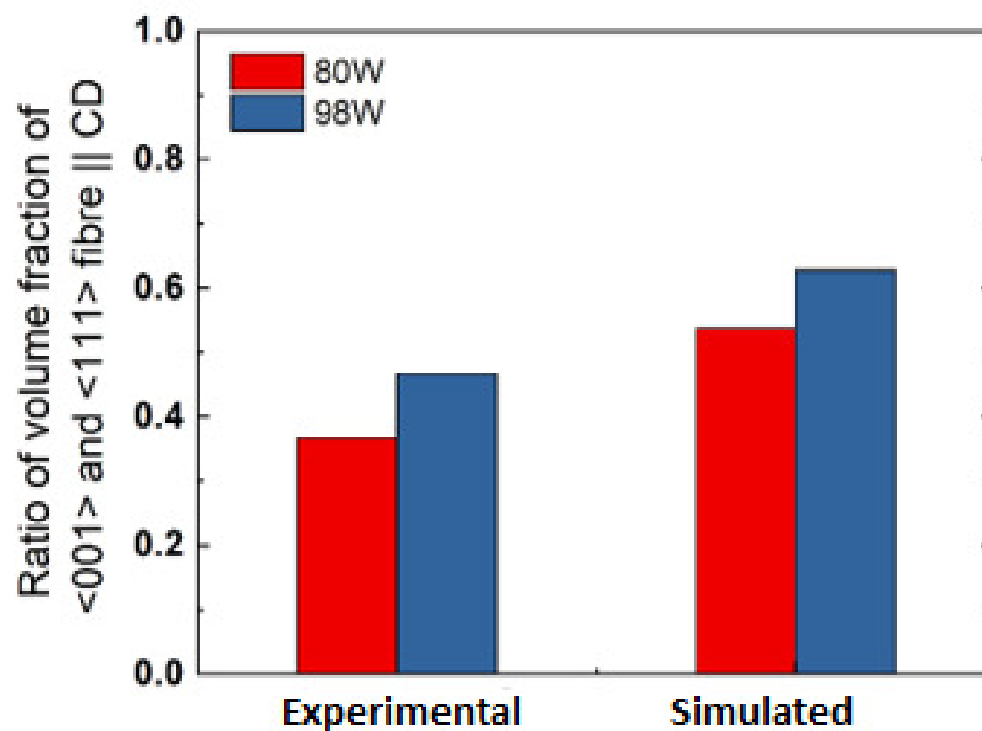
111

001   011

W

Nickel

a) [ī11] [411] [001] [011]

b) 50 μm

SECANT MODEL

Table 1 Composition of tungsten heavy alloy.

Alloy	W (wt.%)	Ni (wt.%)	Fe (wt.%)
80W-20M	80	14	6
85W-15M	85	10.5	4.5
90W-10M	90	7	3
95W-5M	95	3.5	1.5
98W-2M	98	1.4	0.6

Table 2 Parameters for extended Voce hardening law

Phase	Slip system family	τ_0	τ_1	θ_0	θ_1
W	$\{\bar{1}10\} < 111 >$	τ_0	235	355	0
	$\{11\bar{2}\} < 111 >$	$1.3\,\tau_0$	350	100	20
	$\{12\bar{3}\} < 111 >$	$1.5\,\tau_0$	200	100	10
Matrix	$\{111\} < \bar{1}10 >$	$0.6\,\tau_0$	200	100	0

Table 3: Grain size and phase fraction of sintered WHA

Sample	Grain Size of W (μm)	Phase Fraction of Matrix
80W-20M	21 ± 10	0.3
85W-15M	20.7 ± 10.4	0.23
90W-10M	22 ± 13	0.19
95W-5M	20.2 ± 10.3	0.13
98W-2M	20 ± 12	0.08