

# 1 Study on dislocation behavior in a polycrystalline Mg-Y alloy

## 2 using multi-scale characterization and VPSC simulation

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### 19 Abstract

20 In this study, the dislocation behavior of a polycrystalline Mg-5Y alloy during tensile  
21 deformation were quantitatively studied by an in-situ tensile test, visco-plastic self-  
22 consistent (VPSC) modeling, and TEM. The results show that  $\langle a \rangle$  dislocations  
23 contribute to most of the deformation, while a small fraction of  $\langle c+a \rangle$  dislocations are  
24 also activated at near grain boundaries (GBs) regions. The critical resolved shear  
25 stresses (CRSSs) of different dislocation slip systems were estimated. The CRSS ratio  
26 between prismatic and basal  $\langle a \rangle$  dislocation slip in the Mg-Y alloy ( $\sim 13$ ) is lower than  
27 that of pure Mg ( $\sim 80$ ), which is considered as a major reason for the high ductility of  
28 the alloy. TEM study shows that the  $\langle c+a \rangle$  dislocations in the alloy have a high mobility,  
29 which also helps to to accommodate the deformation near GBs.

30 **Keywords:** Mg-Y alloy; dislocation behavior; deformation mechanisms; critical

31 resolved shear stress

32

### 33 **1. Introduction**

34 As the lightest metallic structural material and with big application potential in  
35 aerospace and automotive industries [1, 2], magnesium (Mg) and its alloys have  
36 received strong attention. Nevertheless, due to the limited slip system activated  
37 during deformation, pure Mg and some commercial Mg alloys (e.g., Mg-3Al-1Zn  
38 (AZ31)) have relatively low ductility and formability, which have hindered their  
39 broader applications [3].

40 It has been found that alloying by yttrium (Y) can improve the plasticity of Mg alloys  
41 [4-9]. Sandlöbes et al. [4] reported that a Mg-3Y (wt.%) alloy develops a weak basal-  
42 type texture after rolling and heat treatment, with most grains having their basal plane  
43 (0001) deviate to the rolling plane. Compared to pure Mg (~4%) with strong basal-type  
44 textures, the Mg-3Y alloy shows a distinctively higher tensile elongation (~25%). The  
45 good ductility of Mg-Y alloys, therefore, has been correlated with the weakened  
46 deformation texture by Y [1, 4, 10].

47 The effect of Y on the dislocation **behavior** of Mg plays a key factor as well [5, 11-  
48 17]. Several works regarded the effect of Y on the  $\langle c+a \rangle$  dislocation mobility as the  
49 main mechanism behind [12, 14, 18, 19]. For example, according to the results of  
50 atomistic simulations, Wu and Curtin et al. [12, 20] reported that the cross-slip energy  
51 barrier of the  $\langle c+a \rangle$  dislocation from the pyramidal II to pyramidal I plane in Mg can  
52 be reduced by **an** appropriate Y addition. The reduction **caused** the cross-slip of  $\langle c+a \rangle$   
53 screw dislocations **to become** the main mode of  $\langle c+a \rangle$  dislocation movement. Effective  
54 deformation can be generated by the  $\langle c+a \rangle$  cross-slip, which leads to continuous  
55 dislocation multiplication [11, 12, 21]. Y was also supposed to strengthen the basal  $\langle a \rangle$   
56 dislocation slip in Mg-Y alloys, leading to a **lower** critical resolved shear stress (CRSS)  
57 ratio between non-basal and basal dislocation slip [13, 16, 22, 23]. Kim et al. [13]  
58 investigated the effect of Y on the CRSS values of different dislocation slip in Mg using  
59 molecular dynamics simulation, where the results showed that Y reinforces basal  $\langle a \rangle$

60 dislocation slip more than  $\langle c+a \rangle$  dislocation slip. This can reduce the activation gap  
61 between non-basal slip and basal  $\langle a \rangle$  slip. However, it is yet to reveal whether the Y-  
62 increased mobility of  $\langle c+a \rangle$  dislocation or the Y-strengthened basal  $\langle a \rangle$  slip plays more  
63 important roles in the high ductility of Mg-Y alloys. This can help to reach an in-depth  
64 understanding on the mechanisms of ductility improvement of Mg alloys.

65 Thus, this work **examines** the dislocation **activities** in Mg-Y alloys using in-situ  
66 EBSD/SEM, VPSC simulation, and TEM. The microstructure of a Mg-5Y alloy was  
67 first characterized at different strains by EBSD/SEM. Then the *intragranular* slip traces  
68 and the slip traces *near* grain boundaries (GBs) were investigated separately. The VPSC  
69 modeling was carried out based on the in-situ test results, including the microstructure  
70 evolution, the stress-strain curve, and the measured CRSSs. TEM observation was also  
71 **used to examine** detailed dislocation **behavior**.

72

## 73 **2. Experimental and modeling procedures**

### 74 ***2.1 Sample preparation and characterization***

75 The material used in this work was an extruded Mg-5Y (wt.%) alloy and its process  
76 history has been reported previously [24]. A sample with nominal gauge dimensions of  
77 11 mm (L)  $\times$  4 mm (W)  $\times$  1.4 mm (T) was fabricated by electron discharge machining  
78 for **an** in-situ tensile test, with the tensile direction (TD) being parallel to the extrusion  
79 direction (ED). The sample was electro-polished in an ethanol solution containing 10  
80 vol.% perchloric at 30 V and -30 °C for 150 s. The in-situ tensile test was **conducted** at  
81 room temperature in a SEM (ZEISS, Merlin compact) equipped with an EBSD detector  
82 (Oxford, NordlysMax<sup>2</sup>) and a commercial testing module (Deben, Microtester 2 kN).  
83 The crosshead speed was 0.4 mm  $\cdot$  min<sup>-1</sup>, equivalent to a nominal strain rate of  $6.0 \times 10^{-4}$   
84 s<sup>-1</sup>. SEM was conducted to image the microstructures at strains of 0%, 1.6%, 4.4%,  
85 6.4%, 8.8%, and 12.8%. After each SEM image **collection**, except for 6.4% strain, the  
86 orientation data at different strains was obtained by EBSD characterization. To optimize  
87 the quality of EBSD imaging and the acquisition time, operating voltage of 20 kV and  
88 scan step sizes of 0.5 and 1.0  $\mu$ m were chosen for the EBSD scan. The EBSD data **were**  
89 analyzed by ATEX software v2.01 (<http://www.atex-software.eu/>) and OIM Analysis<sup>TM</sup>

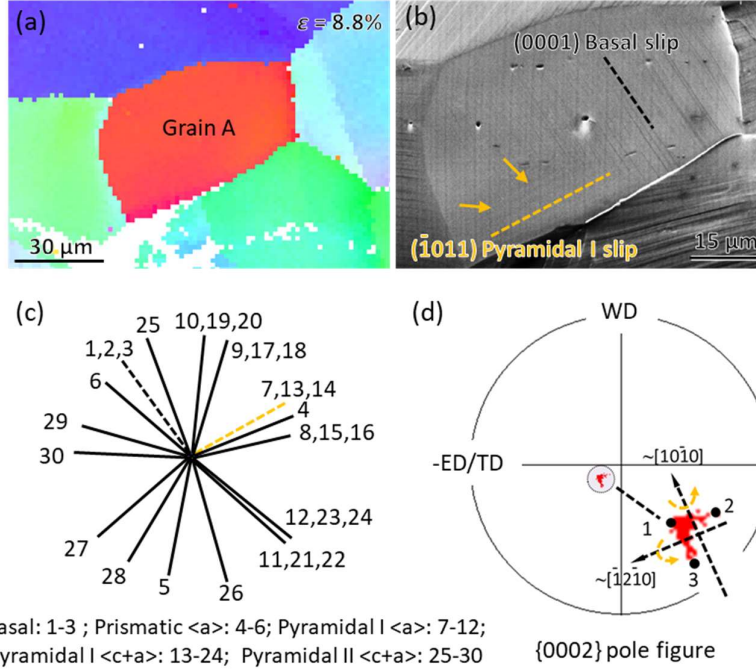
90 v7.0.

91 TEM samples were prepared in an ethanol solution containing 4 vol.% perchloric  
92 acid at 35 V and -40 °C using twin-jet electropolishing (Struers, TenuPol-5). A JEOL-  
93 2100F instrument was operated to image dislocations in grains at working voltage of  
94 200 kV.

95

## 96 ***2.2 Determination of dislocation slip types by lattice rotation analysis***

97 Since the conventional slip trace analysis can only provide limited information of  
98 slip planes [25-27], in this work, a recently developed EBSD-based lattice rotation  
99 analysis was used to determine the types of observed slip traces [24, 28]. Fig. 1 provides  
100 an example for identifying the basal slip system and the pyramidal I slip system. Fig.  
101 1a and 1b show the inverse pole figure (IPF) map and the **corresponding** SEM image  
102 of a region of interest. There are two kinds of surface slip traces in Grain A (Average  
103 Euler angle = (216°, 15°, 314°)). Fig. 1c shows the simulated slip traces of 30 possible  
104 slip systems in the grain (basal  $\langle a \rangle$ : 1-3; prismatic  $\langle a \rangle$ : 4-6; pyramidal I  $\langle a \rangle$ : 7-12;  
105 pyramidal I  $\langle c+a \rangle$ : 13-24; pyramidal II  $\langle c+a \rangle$ : 25-30). A comparison of the observed  
106 slip traces and the simulated slip traces infers that the basal (0001) slip and the  
107 pyramidal I ( $\bar{1}011$ ) slip **systems were** activated. Note that it is difficult to identify their  
108 specific Burgers vectors because all the three basal (i.e., 1, 2, and 3) slip systems share  
109 the same simulated basal slip trace while three pyramidal I (i.e., 7, 13, and 14) slip  
110 systems share the same pyramidal I plane slip trace. In such situations, the Burgers  
111 vectors of the two slip systems **can** be determined based on the long-range intragranular  
112 misorientation of Grain A. Fig. 1d shows the  $\{0002\}$  pole figure of Grain A. An  
113 enlarged image of the (0002) pole shows that the (0002) pole is stretched along two  
114 directions, which represents the lattice rotation of Grain A. Two rotation axes were  
115 determined as  $\sim[10\bar{1}0]$  and  $\sim[\bar{1}2\bar{1}0]$ , respectively, indicating that the slip systems  
116 (0001) $[\bar{1}2\bar{1}0]$  and ( $\bar{1}011$ ) $[\bar{1}\bar{1}2\bar{3}]$  **were** activated in Grain A. The same analysis was  
117 carried out for all the observed slip traces at each deformation step.



118

119 Figure 1. Identification for the activated slip systems by slip trace and lattice rotation analysis. (a) Inverse  
 120 pole figure (IPF) map of Grain A and its neighboring grains. (b) SEM image showing two kinds of surface  
 121 slip traces in Grain A. (c) 30 simulated slip traces of Grain A. (d) {0002} pole figure of Grain A. The (0002)  
 122 pole was stretched along two directions: the streak from 1 to 2 is caused by the basal  $\langle a \rangle$  dislocation slip;  
 123 the streak from 1 to 3 is caused by the pyramidal I  $\langle c+a \rangle$  dislocation slip.

124

### 125 2.3 VPSC modeling

126 In this study, the threshold stress ( $\tau^s$ ) for each slip system ( $s$ ) increasing with  
 127 accumulated shear strain ( $\Gamma$ ) is described by an extended Voce equation:

$$128 \quad \tau^s = \tau_0^s + (\tau_1^s + \theta_1^s \Gamma) (1 - \exp(-\Gamma \frac{\theta_0^s}{\tau_1^s})) \quad (1)$$

129 In the standard VPSC simulation,  $\tau_0^s$ ,  $(\tau_0^s + \tau_1^s)$ ,  $\theta_0^s$ , and  $\theta_1^s$  are the fundamental  
 130 CRSS, the back-extrapolated threshold stress, the initial hardening rate, and the  
 131 asymptotic hardening rate of each deformation mode, respectively. When involving 5  
 132 deformation modes, at least 20 material parameters should be adjusted. Verifying such  
 133 a large number of material parameters is not an easy task.

134 In our work, a simplified approach to VPSC modeling, proposed by Hutchinson et  
 135 al. [29], was adopted. The assumption in Hutchinson's work is that  $\tau_0^s$  indeed involves  
 136 two parts: the fundamental CRSS and a microstructure-related constant ( $\tau_c$ ). The latter  
 137 part derives from the effect of grain boundaries and/or precipitates. Furthermore, for all

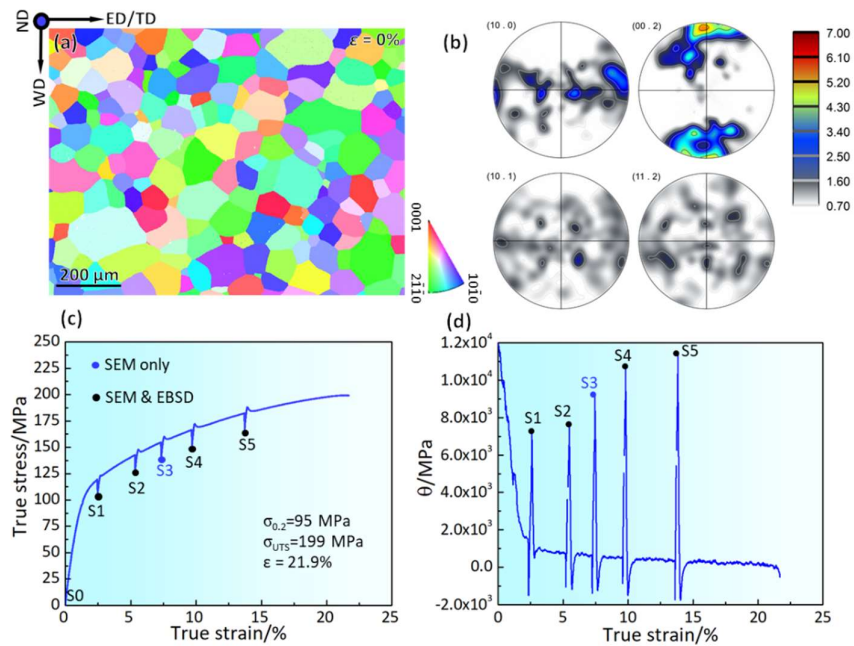
138 deformation modes,  $\tau_c$ ,  $\tau_1^s$ ,  $\theta_0^s$ , and  $\theta_1^s$  were assumed to be constants. This approach  
 139 immensely **reduces** the number of adjustable parameters and has been successfully used  
 140 to predict the complex plastic behavior of AZ31 alloys [29, 30].

141 The initial grain orientations and grain geometry information of 224 grains in the  
 142 Mg-5Y alloy were used as input data for the VPSC modeling. Five deformation modes,  
 143 namely basal  $\langle a \rangle$ , prismatic  $\langle a \rangle$ , pyramidal I  $\langle a \rangle$ , pyramidal I  $\langle c+a \rangle$ , and pyramidal II  
 144  $\langle c+a \rangle$  were included in the simulation. The fundamental CRSSs of different slip modes  
 145 were depended on the experimental CRSSs estimated **from** the in-situ tensile test. The  
 146 **remaining** four parameters (i.e.,  $\tau_c$ ,  $\tau_1^s$ ,  $\theta_0^s$ , and  $\theta_1^s$ ) were determined **by trial and error**  
 147 when a good agreement between the simulated and the experimental results was  
 148 obtained.

149

### 150 3. Results

#### 151 3.1 Initial microstructure



152

153 Figure 2. (a) IPF map of the region of interest before deformation. (b) Pole figures corresponding to (a). (c)  
 154 True stress-true strain curve of the in-situ tensile test during which the SEM/EBSD imaging was conducted  
 155 at 0% (S0), 1.6% (S1), 4.4% (S2), 6.8% (S3, SEM only), 8.8% (S4), and 12.8% (S5) strains. (d) Work  
 156 hardening curve corresponding to the true strain-true stress curve presented in (c). The monotonic decrease  
 157 of the work hardening response was interrupted **during** the in-situ test.

158

159 Fig. 2a and 2b show the microstructure of the Mg-5Y alloy before tensile deformation.  
160 The IPF map of a region with area of  $900\ \mu\text{m} \times 1140\ \mu\text{m}$  (Fig. 2a) and the corresponding  
161  $\{10\bar{1}0\}$ ,  $\{0002\}$ ,  $\{10\bar{1}1\}$ , and  $\{11\bar{2}2\}$  pole figures (Fig. 2b) are presented. The alloy  
162 has a near-equiaxed grain structure with average grain size of  $\sim 96\ \mu\text{m}$ . Because of the  
163 addition of Y, the maximum intensity of the texture component shown in the  $\{0002\}$   
164 pole figure is 5.41 mrd, a value much lower than in some extruded Y-free Mg alloys'  
165 [31-33]. A comparison among the four pole figures indicates that the sample has a less  
166 favorable orientation for basal dislocation slip than for non-basal dislocation slip. The  
167 average macro Schmid Factors (SFs) of the basal  $\langle a \rangle$ , prismatic  $\langle a \rangle$ , pyramidal I  $\langle a \rangle$ ,  
168 pyramidal I  $\langle c+a \rangle$ , and pyramidal II  $\langle c+a \rangle$  dislocation slip in all the grains were  
169 calculated as 0.275, 0.397, 0.445, 0.449, and 0.409, respectively.

170

### 171 **3.2 Tensile deformation at room temperature**

#### 172 **3.2.1 Mechanical properties and microstructure evolution**

173 The true stress-true strain curve of the Mg-Y alloy obtained from the in-situ tensile  
174 test is shown in Fig. 2c. The 0.2% offset tensile yield stress ( $\sigma_{0.2}$ ) and the ultimate tensile  
175 stress ( $\sigma_{UTS}$ ) are 95 MPa and 199 MPa, respectively. As the loading reached the ultimate  
176 tensile stress, the sample failed at a strain of 21.9%. Stress drops occurred at each  
177 probed strain because of the stress relaxation occurring when the tests were paused for  
178 SEM and EBSD imaging. The work hardening curve calculated from the data in Fig.  
179 2c is presented in Fig. 2d. A monotonic decrease of the work hardening rate is apparent,  
180 which implies that no distinct extension twinning occurred during the deformation [35,  
181 36].

182 The grain orientation evolution of the Mg-Y alloy with increasing tensile strain is  
183 presented in Fig. 3. There is no obvious change for the orientation of these grains,  
184 showing that twinning is limited ( $\sim 1.0\%$  in area fraction) before the 12.8% strain. The  
185 low activity of extension twins can be ascribed to the Y addition and the feature of the  
186 extruded texture that most grains are oriented with their  $c$ -axis nearly perpendicular to  
187 the tensile direction [37]. Because the twin volume of the deformed Mg-Y sample is  
188 small, the dislocation behavior focused in this study is under little influence of twinning.

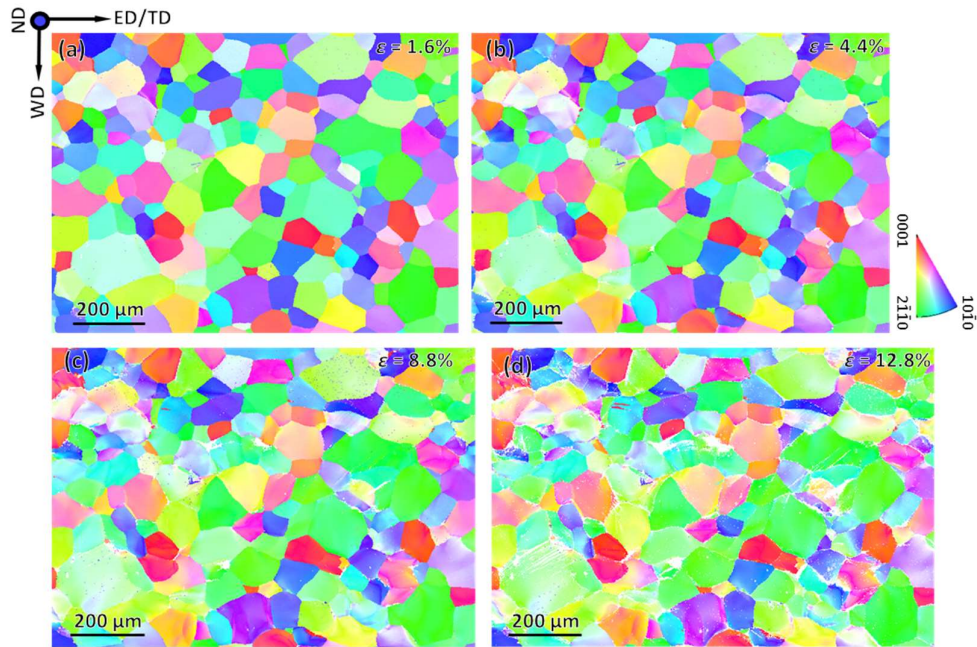
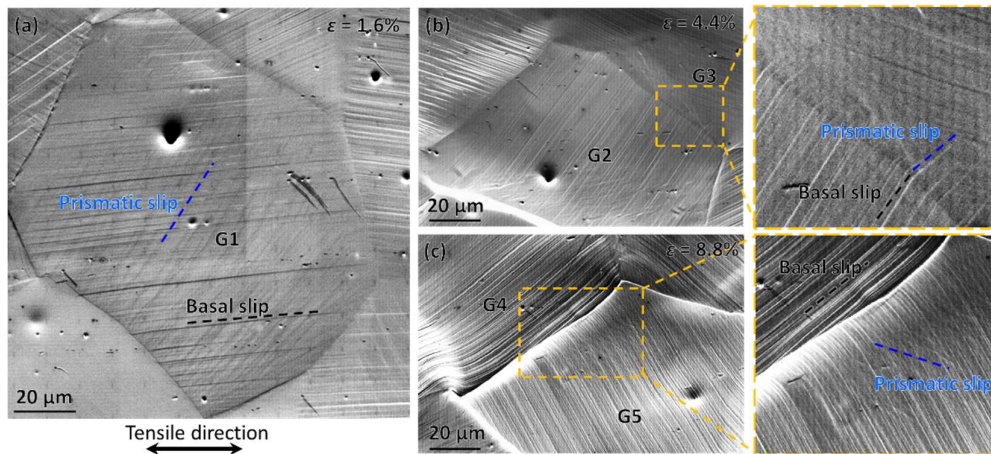


Figure 3. IPF maps showing microstructure evolution with tensile strain.

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### 3.2.2 Non-basal dislocation behavior within grains and near grain boundaries



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Figure 4. Typical morphologies of (a) *intragranular* non-basal slip traces and (b-c) non-basal slip traces *near* GBs.

197 Almost all grains (216 out of 224) developed intragranular basal slip traces even at  
198 1.6% true strain. Fig. 4a shows the slip traces within grain G1 at 1.6% strain. The slip  
199 traces nearly parallel to the TD were determined to be basal slip by slip trace analysis;  
200 the slip traces with an approximately 60° angle to the basal slip traces were from  
201 prismatic slip. Fig. 4b shows that grain G2 is dominated by basal dislocation slip at 4.4%  
202 strain. In grain G3, prismatic slip has been triggered by the basal dislocation slip in



203 grain G2. Fig. 4c shows another type of dislocation slip near GBs: a prismatic slip  
 204 system was locally activated near the GB.

205 To obtain **statistic**, the non-basal dislocation slip traces **inside** grains (such as the  
 206 prismatic slip in Fig. 4a) and **near** GBs (such as the prismatic slip in Fig. 4b and 4c)  
 207 were analyzed at each probed strain for all of the 224 grains in Fig. 2a. As seen in Table  
 208 1, **intragranular** non-basal slip traces are observed in 65, 117, 141, 145, and 155 grains  
 209 at 1.6%, 4.4%, 6.8%, 8.8%, and 12.8% strains, respectively. Non-basal slip traces **near**  
 210 GBs are observed in 54, 81, 92, 94, and 97 grains, respectively. Note that if a grain  
 211 contains more than one type of slip trace, then each type is counted once in Table 1. This  
 212 table shows that prismatic  $\langle a \rangle$  dislocation slip is more dominant than the non-basal  
 213 dislocation slip. This is in agreement with the results of the previous works [7, 38]. The  
 214 statistics in Table 1 also indicates that the fraction of non-basal dislocation slip near  
 215 GBs is comparable to that of the intragranular non-basal dislocation slip. Furthermore,  
 216 it can be inferred that GBs promotes the activation of the pyramidal I  $\langle a \rangle$ , pyramidal I  
 217  $\langle c+a \rangle$ , and pyramidal II  $\langle c+a \rangle$  dislocation slip at the preliminary stage of the tensile  
 218 deformation. For example, at 1.6% strain, the pyramidal I  $\langle a \rangle$ , pyramidal I  $\langle c+a \rangle$ , and  
 219 pyramidal II  $\langle c+a \rangle$  slip traces are observed near 21, 8, and 11 GBs at 1.6% strain, while  
 220 only 9, 1, and 3 grains develop the intragranular pyramidal I  $\langle a \rangle$ , pyramidal I  $\langle c+a \rangle$ ,  
 221 and pyramidal II  $\langle c+a \rangle$  dislocation slip, respectively.

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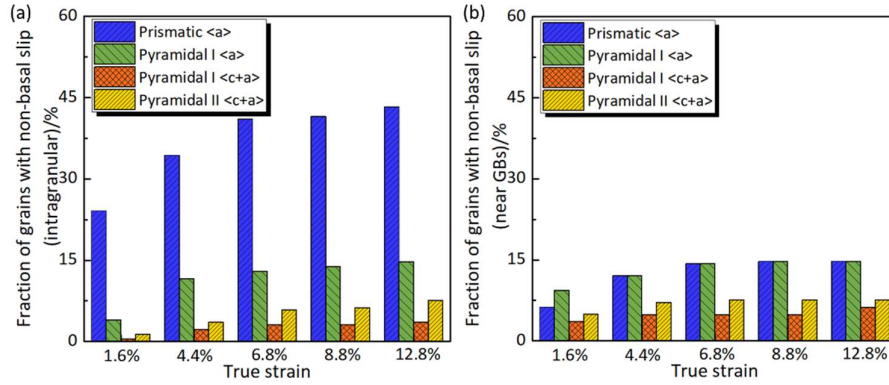
223 Table 1. Slip activity (inside grains and near GBs) for the Mg-5Y sample at various strains.

Strain	Slip modes ( inside grains/near GBs)				Total
	Pris. $\langle a \rangle$	Pyra. $\langle a \rangle$	Pyra. I $\langle c+a \rangle$	Pyra. II $\langle c+a \rangle$	
1.6%	52/14	9/21	1/8	3/11	65/54
4.4%	77/27	26/27	6/11	8/16	117/81
6.8%	92/32	29/32	7/11	13/17	141/92
8.8%	93/33	31/33	7/11	14/17	145/94
12.8%	97/33	33/33	8/14	17/17	155/97

224

225 The fraction of grains with the non-basal slip mode at each deformation strain has  
 226 been calculated as well. Fig. 5a shows that the frequency of the intragranular prismatic  
 227  $\langle a \rangle$  dislocation slip is significantly higher than other intragranular non-basal dislocation

228 slip, suggesting that the CRSS of prismatic  $\langle a \rangle$  dislocation slip is lower than that of  
 229 other types of non-basal dislocation slip in Mg-Y alloy [23]. However, the difference  
 230 in the proportion of different non-basal dislocation slip observed near GB is much  
 231 smaller (Fig. 5b), which indicates that the activation of the non-basal dislocation slip  
 232 around GBs is less sensitive to the macro stress. The stress concentration near GBs  
 233 could play an important role in non-basal dislocation nucleation [39].



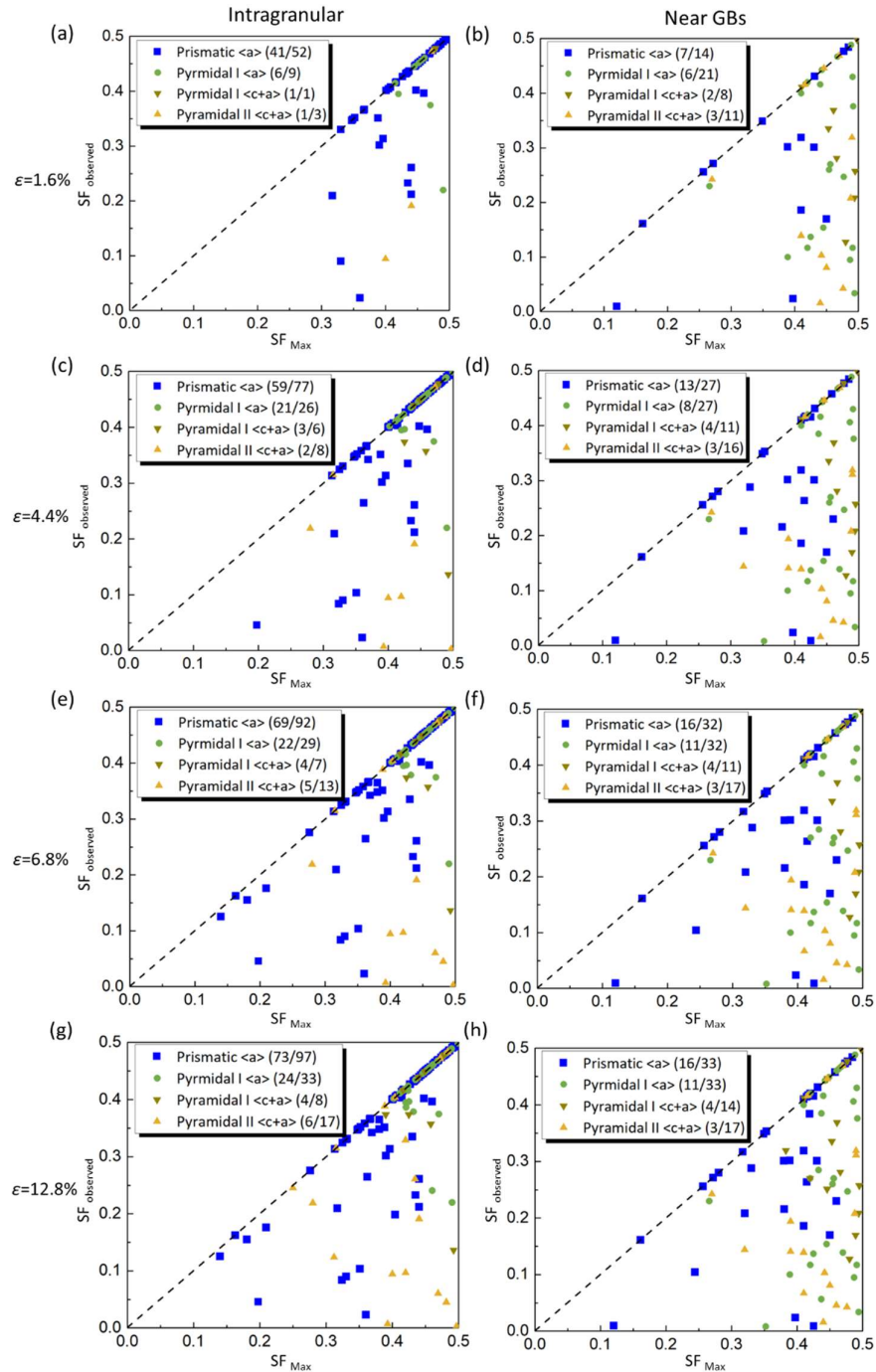
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235 Figure 5. Proportion of grains showing the non-basal dislocation slip traces at different strains for the Mg-  
 236 5Y alloy. (a) Slip traces inside grains and (b) slip traces near GBs.

237

238 Among different slip systems of a slip mode, if the one with the largest SF is activated,  
 239 its activation is always regarded as obeying the Schmid criterion. Conversely, if the  
 240 observed dislocation slip system does not have the largest SF, the activation cannot be  
 241 ascribed merely to the macro stress. To evaluate whether the non-basal dislocation slip  
 242 follow the Schmid criterion or not, the SF of the observed non-basal dislocation slip  
 243 ( $SF_{\text{observed}}$ ) and the maximum SF ( $SF_{\text{max}}$ ) of the corresponding slip mode were  
 244 calculated. Fig. 6a presents the relationship between  $SF_{\text{observed}}$  and  $SF_{\text{max}}$  for the  
 245 intragranular non-basal dislocation slip at 1.6% strain. When  $SF_{\text{observed}}$  and  $SF_{\text{max}}$  are  
 246 the same, data points will be located on the dashed lines. After a close examination, it  
 247 is found that most of data points (43 of 52 prismatic  $\langle a \rangle$ ; 6 of 9 pyramidal I  $\langle a \rangle$ ; 1 of 1  
 248 pyramidal I  $\langle c+a \rangle$ ; 1 of 3 pyramidal II  $\langle c+a \rangle$ ) in Fig. 6a were on the dashed line. Fig.  
 249 6b shows the relationship between  $SF_{\text{observed}}$  and  $SF_{\text{max}}$  for non-basal dislocation slip  
 250 near GBs at 1.6% strain. Much fewer data points (7 of 14 prismatic  $\langle a \rangle$ ; 6 of 21  
 251 pyramidal I  $\langle a \rangle$ ; 2 of 8 pyramidal I  $\langle c+a \rangle$ ; 3 of 11 pyramidal II  $\langle c+a \rangle$ ) in Fig. 6b are  
 252 on the dashed line. A comparison of Fig. 6a and 6b indicates that the activation of most

253 of the intragranular non-basal slip follows the Schmid criterion, whereas only a small  
 254 fraction of the activated dislocation slip near GBs follows the Schmid criterion. This  
 255 confirms that the stress concentration or strain incompatibility near GBs significantly  
 256 affects non-basal dislocation nucleation during deformation.



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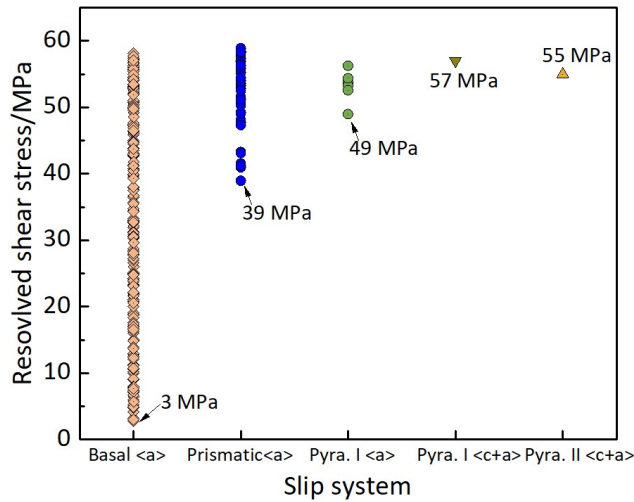
258 Figure 6. Schmid Factors of the activated non-basal dislocation slip ( $SF_{observed}$ ) in comparison to the  
 259 maximum SFs ( $SF_{max}$ ) of the corresponding non-basal slip modes at four strains (in the four rows). The left

260 column presents the observed slips within the grains. The right column presents the the observed slips  
 261 within the grains near GBs, showing that most of the slip near GBs does not follow the Schmid law.

262 Fig. 6c and 6d show the calculated SF values of the activated non-basal dislocation  
 263 slip in comparison to the maximum SF values of the same slip mode at 4.4% strain.  
 264 ~72% of the observed intragranular non-basal dislocation slip has the largest SF, while  
 265 only ~35% of the non-basal slip activation near GBs shows a correlation with the  
 266 Schmid criterion. The same tendency is also observed at higher strains (i.e., 6.8% and  
 267 12.8%), as shown in Fig. 6e-6h.

268

269 **3.2.3 CRSS estimation for the intragranular dislocation slip**



270

271 Figure 7. Experimentally determined shear stresses of the activated dislocation slip in the Mg-5Y alloy.

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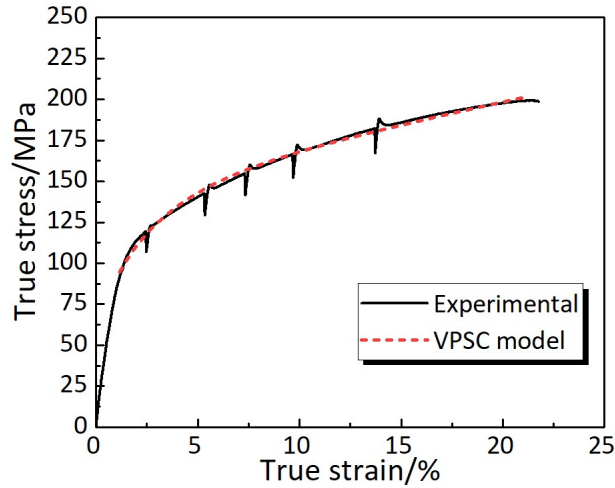
273 **Assuming** that the micro stress of each grain is equal to the macro stress of the tensile  
 274 sample, the resolved shear stresses ( $\tau$ ) acting on the activated intragranular slip system  
 275 can be obtained by  $\tau = \sigma \cdot SF_{\text{observed}}$ , where  $\sigma$  is the applied macro stress [40]. Here, the  
 276 determination for  $\tau$  is based on the observed *intragranular* slip systems that *follow the*  
 277 *Schmid criterion*. Under such conditions, the deformation of these grains was more  
 278 likely controlled by the macro stress. Fig. 7 shows the distribution of the  $\tau$  values of the  
 279 activated slip systems at the macro stress of 118 MPa, corresponding to 1.6% strain. By  
 280 using the minimum resolved shear stress, the CRSS values for the basal <a>, prismatic  
 281 <a>, pyramidal I <a>, pyramidal I <c+a>, and pyramidal II <c+a> dislocation slip are  
 282 calculated as 3 MPa, 39 MPa, 49 MPa, 57 MPa, and 55 MPa, respectively.

283

### 284 3.3 VPSC simulation

285 VPSC modeling based on the in-situ test is a good method to further quantify the  
 286 relative activities of different deformation modes. The true stress-true strain curve  
 287 simulated by the VPSC model is shown in Fig. 8. A good agreement between the  
 288 simulated and experimental strain-stress curves was obtained after a dozen of trials to  
 289 calibrate the material parameters: fundamental CRSSs,  $\tau_c$ ,  $\tau_1^s$ ,  $\theta_0^s$ , and  $\theta_1^s$ . The  
 290 parameters used for the simulation are listed in Table 2. As shown, the CRSS values are  
 291 quite close to the measured values. Fig. 9 compares the simulated deformation texture  
 292 with the experimental measurement. At different strains, the simulated pole figures  
 293 show a good agreement with the experimental results.

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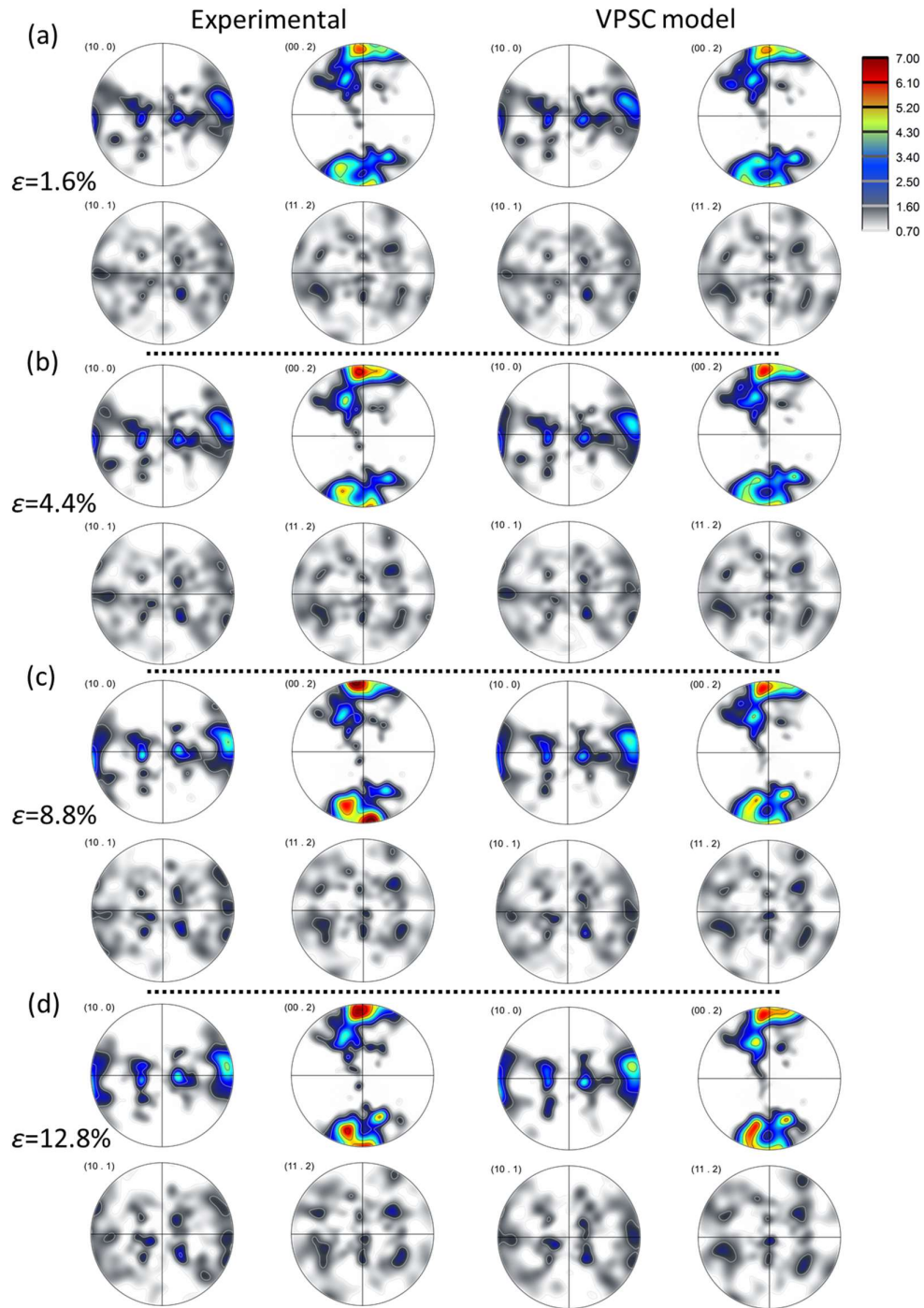
296 Figure 8. Comparison of the simulated true stress-strain curve (the dashed line) by the VPSC simulation  
 297 and the one (the solid line) by the in-situ tensile test shows very close agreement.

298

299 Table 2. Material parameters of the Mg-5Y alloy used in the VPSC modeling (MPa).

Fundamental CRSSs					Adjustable parameters			
Basal <a>	Pris. <a>	Pyra. I <a>	Pyra. I <c+a>	Pyra. II <c+a>	$\tau_c$	$\tau_1^s$	$\theta_0^s$	$\theta_1^s$
2	41	51	72	62	8	15	240	48

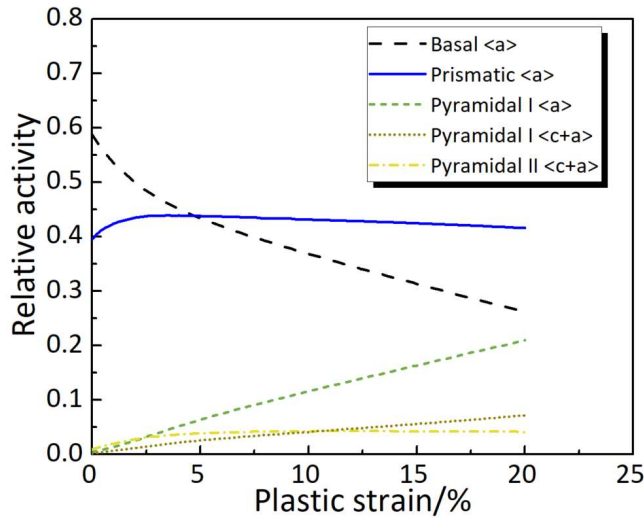
300



301

302 Figure 9. Comparison of the simulated (the left two columns) and the measured (the right two columns)

303 texture for the Mg-Y alloy at (a) 1.6%, (b) 4.4%, (c) 8.8%, and (d) 12.8% strain.



304

305 Figure 10. Simulated relative activity plot for the five slip modes of the Mg-Y alloy as a function of the  
 306 applied strain according to the VPSC simulation.

307

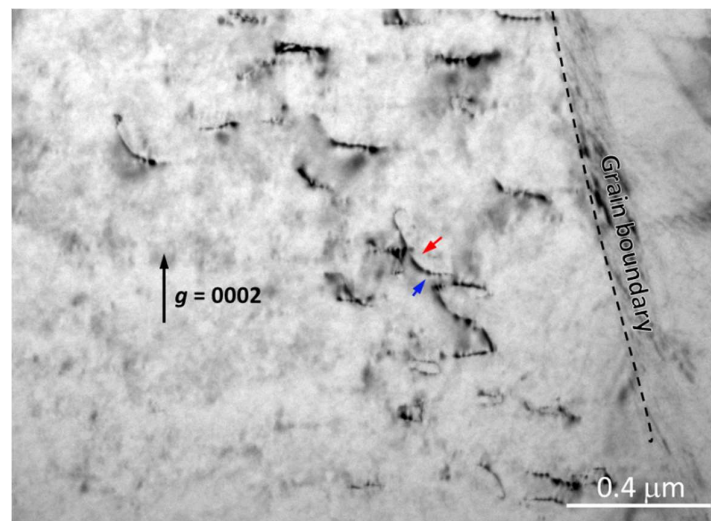
308 Fig. 10 provides the **simulated** relative dislocation activity as a function of plastic  
 309 strains. The results reveal that the tensile deformation in the early stage (< 1.6% strain)  
 310 is dominated by the basal <a> and the prismatic <a> slip modes, which is consistent  
 311 with our experimental observation that the basal <a> and prismatic <a> slip traces are  
 312 **the dominant slip traces**. The simulation also shows that the pyramidal I <a> dislocation  
 313 **activity noticeably increases and** the basal <a> dislocation activity decreases relatively  
 314 with increasing deformation **strain**, but the pyramidal <c+a> dislocation activity keeps  
 315 at a very low level during the deformation. This is in agreement with experimental  
 316 results shown in Fig. 5.

317

### 318 **3.4 TEM observation**

319 Ex-situ TEM observation was performed for 9 grains in a Mg-5Y sample with strain  
 320 of 4%. Based on  $\mathbf{g} \cdot \mathbf{b}$  criterion, where  $\mathbf{g}$  is diffraction vector and  $\mathbf{b}$  is Burgers vector of  
 321 dislocation, it was found that the intragranular deformation of **all 9** grains was  
 322 dominated by <a> dislocations. Some <c+a> dislocations were only observed near GBs.  
 323 Fig. 11 shows a bright-field image of the observed <c+a> dislocations using a  $\mathbf{g} = 0002$   
 324 operating reflection close to the  $[11\bar{2}0]$  zone axis. The dislocation segment marked by  
 325 the blue arrow **is approximately** parallel to **the  $[10\bar{1}0]$  direction**, implying that the <c+a>

326 dislocation slipped on the pyramidal II plane; the dislocation segment marked by the  
327 red arrow has a deviation from the basal plane by  $\sim 60^\circ$ , suggesting that the  $\langle c+a \rangle$   
328 dislocation have slipped on the pyramidal I plane. The L-configuration  $\langle c+a \rangle$   
329 dislocations (7 out of 16  $\langle c+a \rangle$  dislocations) could be a consequence of the cross-slip  
330 of  $\langle c+a \rangle$  dislocation from pyramidal II to pyramidal I plane. Moreover, a close  
331 examination of the dislocation segments shows that the pyramidal II  $\langle c+a \rangle$  dislocations  
332 are of discontinuous dislocation structures, which indicate that the pyramidal II  $\langle c+a \rangle$   
333 dislocations have dissociated. The pyramidal I  $\langle c+a \rangle$  dislocations do not show such a  
334 dissociation phenomenon, which suggests that they have good mobility following  
335 cross-slip in the Mg-5Y alloy.

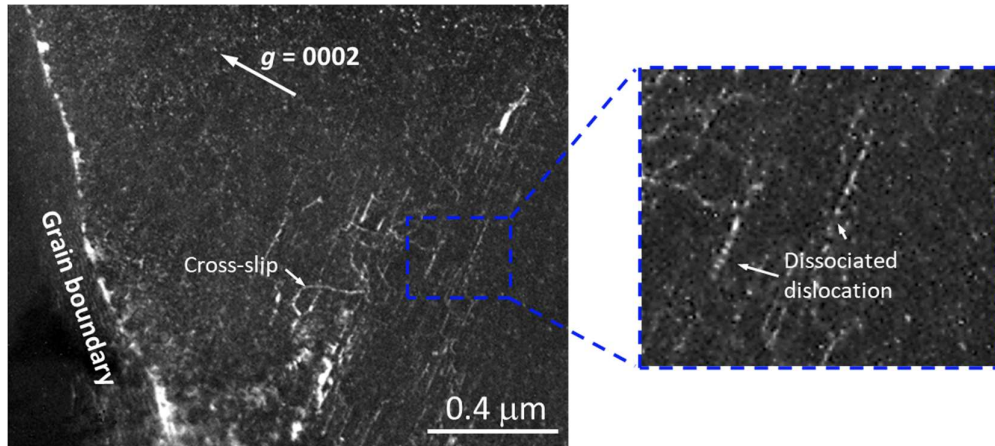


336  
337 Figure 11. Bright-field image for the  $\langle c+a \rangle$  dislocation cross-slip near GB in the Mg-5Y alloy with a 4%  
338 strain, under the  $g = 0002$  diffraction condition near the  $[11\bar{2}0]$  zone axis. The dislocation segment marked  
339 with the blue arrow could be ascribed to the  $\langle c+a \rangle$  dislocation slipped on the pyramidal II plane. The  
340 dislocation marked with the red arrow deviate from the  $[10\bar{1}0]$  by  $\sim 60^\circ$ , suggesting cross-slip occurred.  
341

342 To discover the difference between  $\langle c+a \rangle$  dislocation behavior in Mg alloys with and  
343 without rare-earth elements, an extruded Mg-0.47Ca (wt.%) alloy with an 8% tensile  
344 strain was studied by TEM as well. Fig. 12 presents a dark-field image of  $\langle c+a \rangle$   
345 dislocations taken along the  $[11\bar{2}0]$  zone axis under the  $g = 0002$  operating reflection.  
346 Although  $\langle c+a \rangle$  dislocations can also intensively nucleate near GB in the Mg-Ca alloy,  
347 a large fraction of the  $\langle c+a \rangle$  dislocations (29 out of 40  $\langle c+a \rangle$  dislocations) are linear  
348 without cross-slip behavior. Moreover, the enlarged area shows that the  $\langle c+a \rangle$



349 dislocations have dissociated significantly.



350

351 Figure 12. Dark-field image for the  $\langle c+a \rangle$  dislocation cross-slip near GB in the extruded Mg-0.47Ca  
352 (wt.%) alloy with an 8% tensile strain, under the  $g = 0002$  diffraction condition near the  $[11\bar{2}0]$  zone axis.

353

#### 354 4. Discussion

355 Using the in-situ test in this study, we obtained the CRSSs of different slip modes in  
356 the polycrystalline Mg-Y alloy. The CRSS value of basal  $\langle a \rangle$  dislocation slip in the Mg-  
357 5Y alloy is estimated as 3 MPa, which is larger than that of the pure Mg (0.52 MPa  
358 [41]). An attempt was made to interpret the Y-enhanced  $\text{CRSS}_{\text{basal}\langle a \rangle}$  of the Mg-Y alloy  
359 by Labusch model [42]:

$$360 \quad \Delta\tau = \tau_{\text{alloy}} - \tau_{\text{Mg}} = Kc^{2/3} \quad (2)$$

361 where  $K$  is a constant related to the alloying element and temperature, and  $c$  is the solute  
362 element content, in at. % ( $\sim 1.3$  at.% in this alloy). Based on the  $K$  of the element Y ( $\sim 3$   
363  $\text{MPa}\cdot\text{at}^{-2/3}$ ) as extrapolated in a recent investigation on the solute strengthening effect  
364 in Mg alloys [43], the  $\Delta\tau$  is calculated as 3.4 MPa, which indicates that the  
365 strengthening effect of Y on basal slip generally follows the strengthening model. Thus,  
366 the increase in the  $\text{CRSS}_{\text{basal}\langle a \rangle}$  of the Mg-5Y alloy can be ascribed to solute  
367 strengthening.

368 Reed-Hill et al. [44] reported that the CRSS value of prismatic  $\langle a \rangle$  dislocation slip  
369 in pure Mg is  $\sim 40$  MPa. The  $\text{CRSS}_{\text{prismatic}\langle a \rangle} / \text{CRSS}_{\text{basal}\langle a \rangle}$  ratio of pure Mg therefore can  
370 be calculated as  $\sim 80$ . Based on the measured CRSSs of prismatic  $\langle a \rangle$  and basal  $\langle a \rangle$   
371 dislocation slip in this study, the  $\text{CRSS}_{\text{prismatic}\langle a \rangle} / \text{CRSS}_{\text{basal}\langle a \rangle}$  ratio of the Mg-5Y alloy is

372 calculated as ~13. This indicates that the addition of Y in Mg does reduce the CRSS  
373 ratio between non-basal and basal  $\langle a \rangle$  slips (from 80 to 13). More interestingly, the  
374 CRSS of prismatic  $\langle a \rangle$  in the present alloy is about the same as that of pure Mg alloy.  
375 It implies that addition of Y has selectively strengthened the basal  $\langle a \rangle$  dislocation.  
376 Furthermore, a significant reduction of CRSS ratio of pyramidal  $\langle a \rangle$  and pyramidal  
377  $\langle c+a \rangle$  to basal  $\langle a \rangle$  dislocation slips, all less than 19, is also achieved in the alloy. All  
378 these will contribute to the activation of more non-basal dislocations. In comparison to  
379 the relative activities of different dislocation slips in Mg-0.47Ca alloy [add a reference  
380 here], the fraction of non-basal dislocation slips in the present alloy is much higher. The  
381 difference is especially large for prismatic  $\langle a \rangle$  slips and pyramidal II dislocations. In  
382 the Mg-Ca alloy, the fraction of grains with prismatic  $\langle a \rangle$  slips is less than 20% , while  
383 no pyramidal II dislocations can be observed at tensile strains less than 8%. It clearly  
384 shows the strong effect of Y addition in enhancing non-basal dislocation activities.

385 It has been argued that the improvement effect of Y on  $\langle c+a \rangle$  dislocation mobility is  
386 a more intrinsic mechanism [12, 14, 18-20] for the high ductility of Mg-Y alloys.  
387 Although GBs can enhance the  $\langle c+a \rangle$  dislocation activity in Mg alloys with or without  
388 rare-earth elements due to high stress or strain concentration [39, 45], the activated  $\langle c+a \rangle$   
389 dislocations in Mg alloys without rare-earth elements have relatively poor mobility.  
390 They tend to dissociate into sessile dislocations after nucleation [14], which reduces the  
391 ability to relax the stress concentration near GB. Without effective stress relaxation near  
392 GBs, the stress concentration would lead to premature fracture. In contrast, the stress  
393 concentration could be reduced because of the good mobility of  $\langle c+a \rangle$  dislocations in  
394 Mg alloys with rare-earth elements. The TEM results in the present work does show  
395 that the  $\langle c+a \rangle$  dislocations in the Mg-5Y alloy has higher mobility than that in the Mg-  
396 Ca alloy. Such high mobility  $\langle c+a \rangle$  dislocations, especially those located near GB  
397 regions, will help to accommodate deformation strains, reducing the chance of  
398 premature failure at GBs. However, since the fraction of  $\langle c+a \rangle$  dislocations is rather  
399 low, it is difficult to quantify the contribution of the mobility effect of the dislocations  
400 on the total ductility in the alloys.

401

## 402 **Conclusions**

403 The dislocation slip behavior in an extruded Mg-5Y alloy was systematically  
404 investigated using multi-scale characterization methods. The main results can be  
405 summarized as follows:

- 406 1. The CRSS values of basal  $\langle a \rangle$ , prismatic  $\langle a \rangle$ , pyramidal I  $\langle a \rangle$ , pyramidal I  $\langle c+a \rangle$ ,  
407 and pyramidal II  $\langle c+a \rangle$  dislocation slip in the Mg-5Y alloy were estimated as 3  
408 MPa, 39 MPa, 49 MPa, 57 MPa, and 55 MPa, respectively. The CRSS ratio between  
409 prismatic and basal  $\langle a \rangle$  dislocation slip in the alloy is determined as  $\sim 13$ .
- 410 2. Both experimental and simulation results show that the deformation of the Mg-Y  
411 alloy was dominated by  $\langle a \rangle$  dislocations. The non-basal  $\langle a \rangle$  dislocations shows a  
412 relatively high activity during deformation while the contribution of  $\langle c+a \rangle$   
413 dislocations to the tensile deformation is limited. TEM characterization reveals that  
414 the  $\langle c+a \rangle$  dislocations in Mg-Y alloys have a high mobility due to the ease of  
415 cross-slip.
- 416 3. The high ductility of Mg-Y alloys has been mainly ascribed to the Y-strengthened  
417 basal  $\langle a \rangle$  slip and the significant reduction CRSS ratio between non-basal  
418 dislocations and basal  $\langle a \rangle$  dislocation. The effect of solute Y atoms on mobility  
419 improvement of the  $\langle c+a \rangle$  dislocations is also supposed to contribute to the high  
420 ductility of Mg-Y alloys.

421

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