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# Crystal plasticity modeling of the effects of crystal orientation and grain-to-grain interactions on DSA-induced strain localization in Al–Li alloys

Satyapriya Gupta<sup>a,b,\*</sup>, Vincent Taupin<sup>a,b</sup>, Claude Fressengeas<sup>a,b</sup>, Juliette Chevy<sup>c</sup>

<sup>a</sup>*Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux,  
LEM3, Université de Lorraine/CNRS/Arts et Métiers ParisTech  
7 rue Félix Savart, 57070 Metz, France*

<sup>b</sup>*Laboratory of Excellence on Design of Alloy Metals for low-mAss Structures (DAMAS)  
Université de Lorraine, Nancy-Metz, France*

<sup>c</sup>*C-TEC Constellium Technology Center, 725 Rue Aristide Bergès, Voreppe 38341 cedex, France*

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## Abstract

We develop a crystal plasticity model to investigate the coupled actions of crystal orientation, grain neighborhood and grain-to-grain elasto-plastic interactions on dynamic strain aging (DSA) and the onset and development of associated plastic strain localization in Al–Li alloys. Considering simple model multilayered microstructures with preferred orientations representative of rolled alloys, the aim is to identify grain orientation couples that can limit dynamic strain aging induced strain localization without compromising the flow stress and strain hardening properties. To this end, a slip system-based formulation of dynamic strain aging is implemented in a crystal plasticity finite element framework. The model validity is first checked with the simulation of a tensile specimen loaded at quasi-static applied strain rate. The introduction of dynamic strain aging allows predicting complex propagation of intense plastic localization bands. We further investigate the influence of crystal orientations on early strain localization in Al–Cu–Li–Mg alloys, by performing simulations representative of the early stage of a Kahn Tear test for single crystals and layered polycrystals. Using experimentally reported crystal orientations for rolled microstructures, the simulation results show that in both single and multilayered crystals, there is a strong influence of dynamic strain aging on localization patterns, as well as a significant orientation dependence. In multilayered crystals, the nature of strain localization can be remarkably modified when stand-alone crystals of a certain orientation are coupled with other orientations: strain localization may intensify or fades away depending on the coupling with neighboring orientations.

*Keywords:* Dynamic strain aging; Al–Li alloys; strain localization; grain orientation; crystal plasticity finite element modeling.

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## 1. Introduction

This paper focuses on early plastic strain localization issues in Al–Cu–Li–Mg alloys used as light weight material solutions in the aerospace industry where the primary challenge is to reduce the overall weight of the aircrafts for enhanced fuel efficiency and reduced carbon emission [1–4]. In addition to their low density, these alloys offer an excellent resistance to corrosion and a combination of weldability, mechanical strength and damage tolerance not achieved in conventional alloys [5–7]. However, strain localization phenomena occurring in these alloys which can result into reduced toughness, and the limited understanding of

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\*Correspondence: guptas15@msu.edu; Tel +15174889302

*Email addresses:* guptas15@msu.edu (Satyapriya Gupta), vincent.taupin@univ-lorraine.fr (Vincent Taupin), claude.fressengeas@univ-lorraine.fr (Claude Fressengeas), juliette.chevy@constellium.com (Juliette Chevy)

9 the complex relationships between localization, damage and material properties such as so-  
10 lute/precipitate hardening/softening and crystallographic/morphological texture, still ham-  
11 per their widespread usage [8–10]. Extensive experimental and theoretical efforts have been  
12 made in the recent past for a better understanding of these relationships [11–15].

13

14 In this work, focus is placed on the role of solute strengthening and dynamic strain ag-  
15 ing (DSA) induced Portevin–Le Chatelier (PLC) effect, which is thought to be the primary  
16 phenomena responsible for plastic strain localization in such alloys. In general, PLC effect  
17 is manifested as serrated stress-strain curve and visible strain localizations in the form of  
18 inclined deformation bands and caused by repeated interaction between the moving dislo-  
19 cations and diffusing solute atoms in dilute Al alloys. Although, in contrast to PLC effect,  
20 some precipitates, such as so-called T1 precipitates present in the AA-2198-T8 alloy, were  
21 experimentally suggested to favor homogenization of plastic deformation [16–19], the effect of  
22 precipitation is not considered here and it is left for a forthcoming study. Few experimental  
23 studies explored the role of DSA in the early strain localization processes leading to failure  
24 [20–24], and even fewer discussed the issue in Al–Cu–Li–Mg type alloys [25, 13, 26, 27]. Al-  
25 though such alloys usually do not display the typical serrated stress-strain curves commonly  
26 observed in monotonic uniaxial tensile loading of conventional Al–Mg alloys, recent experi-  
27 mental observations in the AA2024 and AA2139 alloys [28, 29] suggested that DSA could be  
28 activated during interrupted tensile tests, or after jumps in the loading strain rate. Thus, DSA  
29 cannot be ignored in complex forming operations, despite possibly evanescent manifestations  
30 in monotonic loading. Recent in-situ experimental studies combining X-ray laminography  
31 and 3D digital image correlation methods during Kahn tear tests on a AA-2198-T8 rolled  
32 material, and on other similar alloys, clearly evidenced the occurrence of early plastic strain  
33 localization [13, 30]. It was observed that intense plastic localization bands form away from  
34 the crack tip at the very beginning of deformation, and these bands are intermittent in time  
35 but not in space. This is very detrimental as plastic deformation will accumulate in bands,  
36 which inevitably leads to fracture of the specimens due to progressive void nucleation and  
37 coalescence at intermetallic particles in these slanted bands. By performing Kahn tear tests  
38 simulations using a finite element model that couples crystal plasticity, dynamic strain aging,  
39 damage and fracture, it was affirmative that dynamic strain aging is responsible for these  
40 early strain localization phenomena [26]. Localization bands intermittent in time but less  
41 in space were indeed predicted in good agreement with experimental data, which lead to  
42 damage and eventual fracture of the samples.

43

44 Motivated by the above studies [13, 30, 26], present work contributes to further investiga-  
45 tion in terms of modeling the role of crystal orientations, plastic anisotropy, grain neighbor-  
46 hood, and grain-to-grain interactions on the intensity of dynamic strain aging effects. In a  
47 recent study, simple model lamellar grain structures representative of rolled microstructures  
48 were modeled, using experimentally reported preferred crystal orientations [31]. Plastic het-  
49 erogeneity and anisotropy was observed in the simulations. Such anisotropy and a significant  
50 soft-stiff grain-to-grain contrast was further reported both experimentally and theoretically  
51 in similar Al–Li rolled alloys [32–34], where in particular Brass and S orientations exhibit a  
52 strong stiff-soft behavior contrast. As such, with the eventual aim of minimizing or avoiding  
53 the detrimental effects of DSA on strain localization and the subsequent fracture process of  
54 Al–Cu–Li–Mg alloys through adequate material design, we strive to understand how DSA  
55 interacts with typical crystallographic and morphological orientation patterns. In the present  
56 work, we probe these interactions using a crystal plasticity finite element (CPFE) model. For  
57 capturing the key features of these interactions, a slip system-based dynamic strain aging  
58 module is added to the modeling framework. In studying the roles of grain morphology  
59 and orientation on strain localization, experimentally observed layered microstructures and  
60 dominant crystal orientations are employed. More precisely, we will perform simulations  
61 representative of the early stage deformation of a Kahn tear test, considering first, single

Table 1: Grain orientations used in the simulations. The Euler angles  $(\phi_1, \phi, \phi_2)$  (in  $^\circ$ ) provide the orientation of the crystal with respect to the rolling frame.

| <i>Orientation</i> | $\phi_1$ | $\phi$ | $\phi_2$ |
|--------------------|----------|--------|----------|
| Brass-b            | 35.26    | 45.0   | 0.0      |
| S-d                | -121.02  | 143.3  | 26.57    |
| Cube               | 0.0      | 0.0    | 0.0      |
| Goss               | 0.0      | 45.0   | 0.0      |
| TCX                | 72.9     | 22.6   | 36.9     |

62 crystals and specific orientations (see Table 1). In particular we have considered a variant of  
 63 the Brass texture component (called Brass-b hereafter), a variant of the S texture compo-  
 64 nent (presented as S-d hereafter), Cube and Goss texture components, as well as an unknown  
 65 texture component X (will be called TCX hereafter).

66 As we neglect precipitation here, the material modeled can be considered as a AA-2198-  
 67 T3 type alloy instead of the AA-2198-T8 alloy, where strong nanosize precipitates have  
 68 been formed during additional aging. The aim is not to fit as close as possible available  
 69 experimental curves here, but rather to identify which orientations are better in terms of  
 70 limiting plastic strain localization initiating at the crack tip and very quickly propagating  
 71 through the material and in terms of flow stress and strain hardening. Second, based on  
 72 lamellar structures typical of 2198, we will simulate the same test for model microstructures  
 73 with two major grain orientations, for instance, stacks of alternate Brass-b and S-d lamellar  
 74 grains will be modeled and simulated. This study tries to be useful in terms of materials  
 75 design as it allows probing the effect of coupling a given orientation with other neighboring  
 76 orientations on the plastic heterogeneity and anisotropy.

77 The following sections of the paper are therefore organized as follows. The small strain  
 78 crystal plasticity framework accounting for DSA is presented in Section 2. Proper working  
 79 of the DSA-embedded CPFEE model is numerically validated in Section 3. CPFEE simulation  
 80 results obtained for different crystal orientations and several layered morphologies of orien-  
 81 tation couples are presented and discussed in Section 4 . Finally, conclusions of the work are  
 82 listed in Section 5.

## 83 2. DSA-enabled CPFEE model

84 The unknown field is the displacement field  $\mathbf{u}$  in a body  $B$  subjected to displacement  
 85 and/or traction boundary conditions. In the absence of inertial and body forces, the momen-  
 86 tum balance equation and boundary conditions can be written as

$$\mathbf{div} \mathbf{T} = 0 , \quad (1)$$

$$\mathbf{T} \cdot \mathbf{n} = \bar{\mathbf{t}} \text{ on } S_t , \quad (2)$$

$$\mathbf{u} = \bar{\mathbf{u}} \text{ on } S_u , \quad (3)$$

87 where  $\mathbf{T}$  is the stress tensor and  $(\bar{\mathbf{t}}, \bar{\mathbf{u}})$  are prescribed tractions and displacements at external  
 88 boundaries of unit normal  $\mathbf{n}$ , respectively. Homogeneous linear isotropic elasticity of the  
 89 material is assumed:

$$T_{ij} = \lambda \epsilon_{kk}^e \delta_{ij} + 2\mu \epsilon_{ij}^e. \quad (4)$$

90 In this relation,  $\lambda$  and  $\mu$  are the Lamé constants, and  $\epsilon^e$  the elastic strain tensor. In a small  
 91 strain setting,  $\epsilon^e = \epsilon - \epsilon^p$ , where  $\epsilon$  and  $\epsilon^p$  are the total and plastic strain tensors.

92 *2.1. Crystal plasticity module*

93 In the present crystal plasticity model, we follow the formulation used for aluminium  
94 crystals in [35]. The plastic velocity gradient  $\mathbf{L}_p$  (whose symmetric part is the plastic strain  
95 rate tensor  $\dot{\boldsymbol{\epsilon}}^p$ ) is obtained in a classical manner from the summation of the shear rates arising  
96 from dislocation glide on all activated slip systems:

$$\mathbf{L}_p = \sum_s \dot{\gamma}_s \mathbf{P}_s = \sum_s \rho_s^m b v_s \mathbf{m}_s \otimes \mathbf{n}_s. \quad (5)$$

97 In this relation,  $\mathbf{P}_s = \mathbf{m}_s \otimes \mathbf{n}_s$  is known as the orientation Schmid tensor of the slip system  $s$   
98 with slip direction  $\mathbf{m}_s$  and unit normal  $\mathbf{n}_s$ . The shear rate  $\dot{\gamma}_s$  on the slip system  $s$  is given by  
99 the Orowan relationship  $\dot{\gamma}_s = \rho_s^m b v_s$ , where  $b$  is the magnitude of the Burgers vector on all  
100 slip systems,  $\rho_s^m$  denotes the mobile dislocation density and  $v_s$  is the dislocation velocity on  
101 slip system  $s$ . The plastic slip on system  $s$  is driven by the resolved shear stress  $\tau_s = \mathbf{T} : \mathbf{P}_s$   
102 through the power law relationship

$$v_s = v_0 \left( \frac{|\tau_s|}{\tau_s^h + \tau_s^{sol}} \right)^n \text{sgn}(\tau_s) \quad (6)$$

103 reflecting hardening from thermally activated obstacle overcoming, where  $v_0$  is a reference  
104 velocity and  $n$  a power law exponent. The stress  $\tau_s^h$  reflects forest hardening on the slip  
105 system  $s$ , and is assumed to be of the following form:

$$\tau_s^h = \mu b \sqrt{\sum_j a_{js} \rho_j^f}, \quad (7)$$

106 where  $a_{js}$  is a latent hardening coefficient providing the contribution of the dislocation forest  
107 density  $\rho_j^f$  on system  $j$  to the hardening of system  $s$  [36]. A mean value  $a_{mean}$  will be taken  
108 for all these coefficients, except for the collinear interactions where the (larger) value  $a_{col}$  will  
109 be used. In the provisional absence of DSA, the rates of change of the mobile  $\rho_s^m$  and forest  
110  $\rho_s^f$  dislocation densities on slip system  $s$  are taken as

$$\frac{\dot{\rho}_s^m}{\rho_0^m} = \left( K_m - K_f + \frac{C_1}{\sqrt{\rho_0^m}} \sum_j \sqrt{\rho_j^f} - \frac{C_2}{\rho_0^m} \sum_j \sqrt{\rho_s^m \rho_j^f} \right) |\dot{\gamma}_s|, \quad (8)$$

$$\frac{\dot{\rho}_s^f}{\rho_0^m} = \left( K_f + \frac{C_2}{\rho_0^m} \sum_j \sqrt{\rho_s^m \rho_j^f} - \frac{C_3}{\rho_0^m} \rho_s^f \right) |\dot{\gamma}_s|. \quad (9)$$

111 In the above,  $K_m$  is connected with the multiplication and  $K_f$  with the immobilization of  
112 mobile dislocations on obstacles initially present in the crystal.  $C_1$  reflects the contribution  
113 of the forest dislocations to mobile dislocation sources.  $C_2$  accounts for the immobilization of  
114 mobile dislocations due to their interactions with the forest.  $C_3$  stands for dynamic recovery.  
115  $\rho_0^m$  is a reference dislocation density value. By handling separately the dislocation densities  
116 on each slip system, these evolution laws are designed to account for the effects of crystal  
117 orientation on the flow stress and work hardening rate [35]. In addition, Eq.(8) is meant to  
118 reflect the quick increase and saturation of the mobile dislocation density on an activated  
119 slip system.

120

121 *2.2. Dynamic strain aging module*

122 In Eq.(6),  $\tau_s^{sol}$  is an additional hardening stress arising from DSA, *i.e.*, from recurrent  
123 pinning by diffusing solute atoms and eventual breakaway of mobile dislocations arrested  
124 on their obstacles. Its evolution with the aging time of arrested dislocations and the solute

125 concentration at these dislocations is now described, together with their effects on the dislo-  
 126 cation density evolutions. A slip-system based Kubin Estrin McCormick (KEMC) model was  
 127 recently applied to Al-Cu-Li-Mg alloys [26]. Here, as our crystal plasticity model couples the  
 128 evolution of both mobile and forest dislocation densities, we consider another dynamic strain  
 129 aging constitutive model that also distinguish the dynamics of mobile and sessile dislocation  
 130 densities [37]. The chosen DSA module couples the time evolution of mobile and forest dis-  
 131 location densities  $(\rho_s^m, \rho_s^f)$  with the variations of the aging time  $t_s^a$  and solute concentration  
 132  $C_s^{sol}$  at arrested dislocations on particular slip system  $s$ . To this aim, the equations (8,9) are  
 133 augmented as follows:

$$\frac{\dot{\rho}_s^m}{\rho_0^m} = \left( K_m - K_f + \frac{C_1}{\sqrt{\rho_0^m}} \sum_j \sqrt{\rho_j^f} - \frac{C_2}{\rho_0^m} \sum_j \sqrt{\rho_s^m \rho_j^f} \right) |\dot{\gamma}_s| - \frac{A_1}{t_s^l} \rho_s^m p(\dot{\gamma}_s), \quad (10)$$

$$\frac{\dot{\rho}_s^f}{\rho_0^m} = \left( K_f + \frac{C_2}{\rho_0^m} \sum_j \sqrt{\rho_s^m \rho_j^f} - \frac{C_3}{\rho_0^m} \rho_s^f \right) |\dot{\gamma}_s| + \frac{A_1}{t_s^l} \rho_s^m p(\dot{\gamma}_s). \quad (11)$$

In Eqs.(10,11), the effects of DSA on the time evolution of the dislocation densities are taken into account through the terms involving  $A_1$ , as they effectively integrate the dynamics of dislocations and solute atoms. These terms control the exchange of dislocations between  $\rho_s^m$  and  $\rho_s^f$  by arrest and breakaway of mobile dislocations in relation with solute diffusion. The characteristic time  $t_s^l$  (also called loading time) are defined from the elementary incremental strain  $\Omega_s$  and the overall loading strain rate  $\dot{\epsilon}_a$ :

$$t_s^l = \frac{\Omega_s}{\dot{\epsilon}_a} = \frac{b \bar{\rho}_s^m / \sqrt{\bar{\rho}_s^f}}{\dot{\epsilon}_a}. \quad (12)$$

The incremental strains  $\Omega_s$  depend only on the slow time scale evolutions of  $\rho_s^m$  and  $\rho_s^f$ , as determined from Eqs.(8,9) and denoted  $(\bar{\rho}_s^m, \bar{\rho}_s^f)$ , but the characteristic times  $t_s^l$  set the time scales for the fast dislocation dynamics associated with DSA.  $p(\dot{\gamma}_s)$  represents the probability density for dislocations to get pinned at obstacles by clouds of solute atoms on slip system  $s$ . Expressed in terms of the plastic strain rate  $\dot{\gamma}_s$ , it reflects the elastic dislocation-solute interactions on slip system  $s$  and can be taken as

$$p(\dot{\gamma}_s) = \frac{2\dot{\gamma}_s}{\dot{\epsilon}_0^2} \exp(-(\dot{\gamma}_s/\dot{\epsilon}_0)^2). \quad (13)$$

134 where the reference strain rate  $\dot{\epsilon}_0$  is an input parameter regulating the type of serration  
 135 achieved from the model. In the presence of DSA, a switch occurs repeatedly between low  
 136 and high solute concentration  $C_s^{sol}$  along the master curve described in Eq.(14) as a function  
 137 of the dislocation aging time  $t_s^a$ .

$$C_s^{sol} = 1 - \exp\left(-\left(\frac{t_s^a}{t_D}\right)^{2/3}\right) \quad (14)$$

138 In relation (14),  $t_D$  is a time scale characterizing solute diffusion. The switch is therefore  
 139 controlled by the aging time, which in turn primarily depends on the magnitude of the local  
 140 plastic strain rate  $\dot{\gamma}_s$ . In the model [37], this switch is achieved through a relaxation process,  
 141 according to which the aging time  $t_s^a$  follows the waiting time  $t_s^w$  (mobile dislocations wait  
 142 on their obstacles in slip system  $s$ ) with some delay:

$$\frac{dt_s^a}{dt} = 1 - \frac{t_s^a}{t_s^w} \quad (15)$$

$$t_s^w = \frac{\Omega_s}{|\dot{\gamma}_s|}. \quad (16)$$

143 Hence, the PLC instability occurs when the waiting time  $t_s^w$ , which indirectly depends on  
 144 the flow stress, drops down to zero, reflecting the unpinning of dislocations from solute  
 145 atmospheres. The solute-related resistance  $\tau_s^{sol}$  on slip system  $s$  is now taken as the product  
 146 of the solute concentration  $C_s^{sol}$  on arrested dislocations and a saturation stress level  $f$  reached  
 147 at large aging times  $t_s^a$ :

$$\tau_s^{sol} = fC_s^{sol} . \quad (17)$$

148 Note that all the CP and DSA material parameters are listed in Table 2. The parameters  
 149 for DSA and latent hardening are taken from previous works [38, 37, 35].

### 150 2.3. Numerical strategy

151 The standard Galerkin finite element method is used for the spatial discretization and  
 152 numerical solution of the problem set out by Eqs.(3) through (17). Note that the differential  
 153 equations and relations (10-17) presented above constitute a stiff differential system involving  
 154 fast variables undergoing large changes in a small amount of time. An explicit time-marching  
 155 scheme is employed with sufficiently small time steps, to ensure numerical stability of the  
 156 solution. The choice of time step  $\Delta t$  is chosen based on limited relative evolution of both  $\mathbf{L}_p$ ,  
 157  $t_s^a$  and  $\dot{\gamma}_s$  quantities. The model is implemented in the framework provided by Freefem++,  
 158 a free software based on the finite element method having a high level integrated develop-  
 159 ment environment for the numerical solution of partial differential equations in two or three  
 160 dimensions [39].

## 161 3. DSA endorsed strain localization in single crystal tension: validation of model

162 Single crystal stretching simulations are performed using the above described DSA-  
 163 enabled model to examine the proper working, capabilities and flexibility of the CPFE code.  
 164 The simulation results are compared with conventional CP response to highlight the influ-  
 165 ence of DSA on the mechanical response. A classical dog bone-shaped sample is simulated  
 166 with uniaxial tension velocity driven boundary conditions in the X direction. Note that  
 167 X,Y,Z in FE model correspond to RD,TD and ND. The FE domain (generated by the mesh  
 168 module of Freefem++) is discretized with cubes composed of tetrahedral elements and the  
 169 crystal lattice is assigned Euler angles characteristic of the cubic orientation, typically close  
 170 to experimentally used orientations in tensile samples. The material properties and initial  
 171 condition parameters used for the simulations are listed in Table 2. The applied strain rate  
 172 is  $10^{-4}/s$ . In all forthcoming simulations, the mesh is chosen fine enough such that realis-  
 173 tic plastic localization bands can develop. However, in a more realistic setup, one should  
 174 consider strain gradient plasticity or field dislocation mechanics [40] approaches, where a  
 175 characteristic internal length scale related to width of localization bands can be explicitly  
 176 or inherently introduced to remove any mesh size dependence of the plastic bands [41]. In  
 177 our simulations, there is no physical size introduced, only the effect of grain morphologies,  
 178 its distribution and the ratio of lamellar grain thicknesses in our multilayered simulations is  
 179 important.

180  
 181 Two different regimes of plastic activity were observed. Fig. 1(a) shows a zoomed-in view  
 182 of the macroscopic stress-strain curve obtained from the DSA-enabled model featuring a se-  
 183 quence of irregular events, which can be compared with the very smooth curves obtained  
 184 from conventional CP modeling in Fig. 1(b). The magnitude of the stress serrations is very  
 185 small (which is realistic for Al-Cu-Li-Mg alloys) for the adopted DSA parameters. In ad-  
 186 dition, a higher flow stress (an increase of the yield stress of about 50 MPa) together with  
 187 larger yield drop is observed for DSA-enabled model as compared to the conventional CP  
 188 model. This is due to the fact that, in the latter case, the yield point originates in a burst of  
 189 the mobile dislocation density (due to very small initial mobile dislocation densities  $\rho_s^m(0)$ ),

190 whereas the former case also involves the breakaway of statically aged mobile dislocations.

191

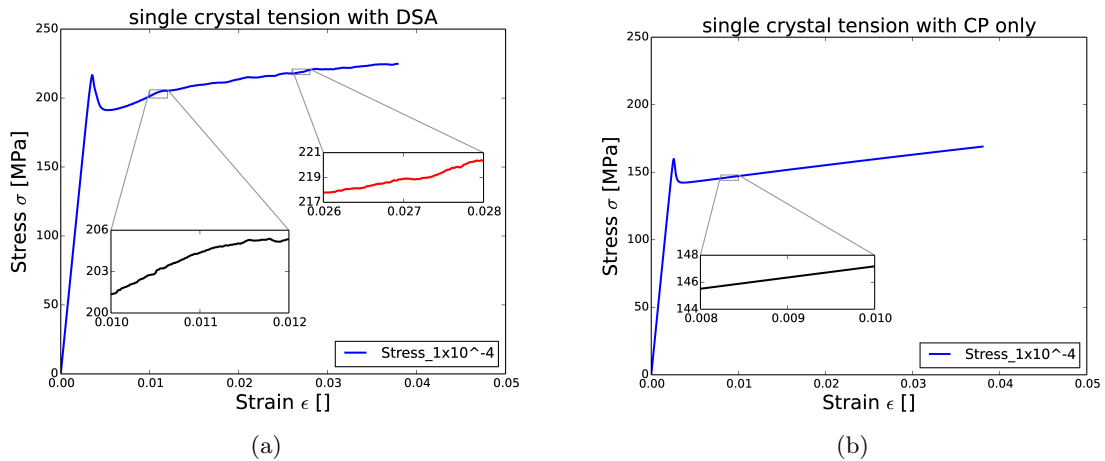


Figure 1: Macroscopic deformation behavior of dogbone-shaped single crystal in tension, (a) with DSA enabled crystal plasticity; (b) In the absence of DSA (crystal plasticity only).

192 The simulation results are also analyzed at a more local level using the longitudinal  
 193 strain rate fields (primarily plastic strain rate) obtained from both the DSA-enabled CP  
 194 and conventional CP models. The dogbone shape of the simulated sample provides natural  
 195 opportunity for stress concentration at the shoulders, and thereby a region to initiate strain  
 196 localization. As shown in Fig. 2(a), nucleation, motion and intermittency of strain localiza-  
 197 tion in the form of bands can be observed in the DSA-enabled model. For instance, a closer  
 198 look on the maps at time steps (ts) 190, 250, and 300 demonstrates the formation of two new  
 199 bands at the specimen shoulders and disappearance of the band in the middle of the mesh.  
 200 The manifestations of these plastic instability events are clearly the attributes of repeated  
 201 collective pinning and breakaway of mobile dislocations.

202

203 On the contrary, strain localization is completely absent from the strain rate fields ob-  
 204 tained from the conventional CP model (see Fig. 2(b)), which confirms the proper working  
 205 of the DSA-enabled model and also highlights the influence of DSA on the local deformation  
 206 behavior of the material. We indeed observe a very homogeneous strain rate field throughout  
 207 the gauge length of the specimen in Fig. 2(b). The initial burst of mobile dislocations due to  
 208 low initial mobile dislocation densities  $\rho_s^m(0)$  is seen to temporarily fill up the gauge length  
 209 with high strain rate.

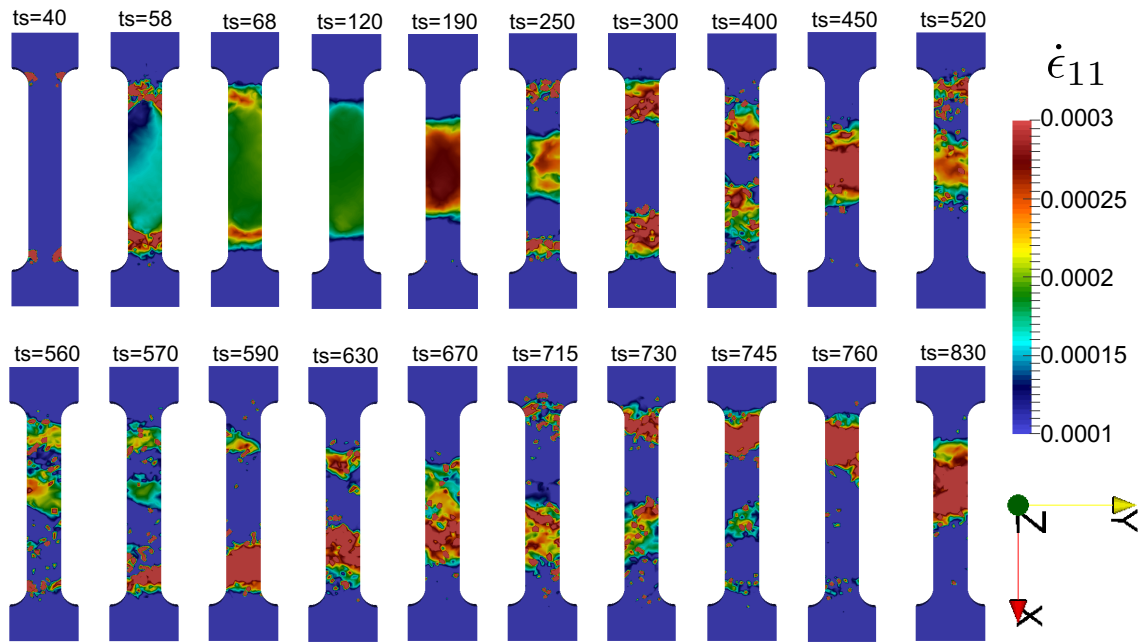
#### 210 4. Strain localization in Al–Cu–Li–Mg alloys: Influence of crystal orientation and 211 morphological texture

212 As already mentioned, the present study is grounded on the presumption that strain  
 213 localization is a middle link of deformation and ultimate fracture. Strain localization is  
 214 therefore the primary focus of our investigation. The following study is conducted to investi-  
 215 gate how the crystal orientation and layered morphology can influence the strain localization  
 216 process ahead and away from a crack tip in the presence of DSA. In the bigger picture, this  
 217 investigation aims at tailoring a textured alloy, in order to make it less susceptible to strain  
 218 localization and thus to have better damage/fracture resistance.

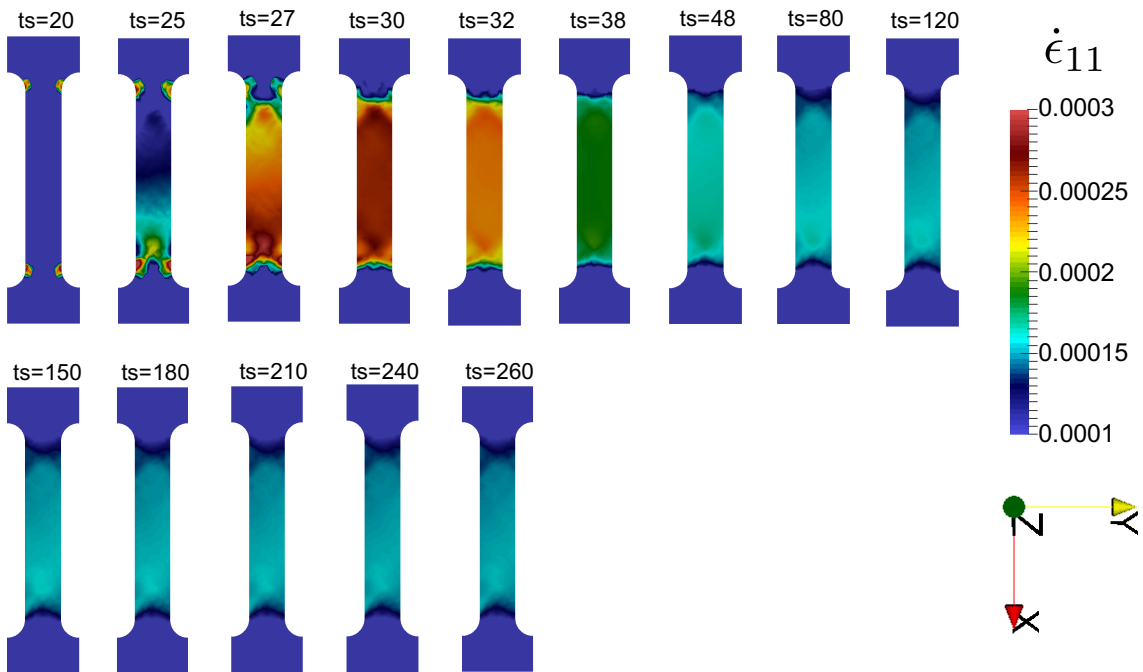
##### 219 4.1. Edge cracked single crystal: effect of crystal orientation

220 The simulation results presented in the previous section demonstrate that DSA can trig-  
 221 ger plastic instabilities in dilute Al alloys, which are otherwise absent when DSA is omitted.





(a)



(b)

Figure 2: Longitudinal strain rate field  $\dot{\epsilon}_{11}$  at gradually increasing simulation time steps for the dog bone-shaped single crystal (a) simulated with DSA enabled crystal plasticity where destabilizing influence of DSA is manifested in the form of the nucleation, motion and intermittency of localized deformation bands; (b) simulated with crystal plasticity in the absence of DSA (standard CP model) where the complete absence of plastic instability and localized bands with a homogeneous strain rate field across the gauge section highlights the significant influence of DSA.

Table 2: Material and simulation parameters used for crystal plasticity (CP) and dynamic strain aging (DSA).

| <b>CP model parameters</b>             | <b>Notation</b>    | <b>Value</b>                     |
|--|--------------------|----------------------------------|
| Power law exponent                     | $n$                | 10                               |
| Reference dislocation velocity         | $v_0$              | $5 \times 10^{-10} \text{m/s}$   |
| Reference mobile dislocation density   | $\rho_0^m$         | $1 \times 10^7 \text{m}^{-2}$    |
| Latent hardening coefficients          | $a_{mean}$         | 0.12                             |
|  | $a_{col}$          | 1.265                            |
| Burgers vector magnitude               | $b$                | $2.86 \times 10^{-10} \text{m}$  |
| Dislocation interaction with obstacles | $K_m$              | $2.4 \times 10^4$                |
|  | $K_f$              | $1.4 \times 10^4$                |
| Hardening/softening parameters         | $C_1$              | $2.2 \times 10^3$                |
|  | $C_2$              | 80.0                             |
|  | $C_3$              | 0.0                              |
| Lamé constants                         | $\lambda$          | 62 GPa                           |
|  | $\mu$              | 23 GPa                           |
| <b>DSA model parameters</b>            | <b>Notation</b>    | <b>Value</b>                     |
| Diffusion time                         | $t_D$              | 10 sec                           |
| Arrest term                            | $A_1$              | $1 \times 10^{-3} \text{s}^{-1}$ |
| Solute hardening constant              | $f$                | 37 MPa                           |
| Reference strain rate                  | $\dot{\epsilon}_0$ | $5 \times 10^{-4} \text{s}^{-1}$ |
| Applied strain rate                    | $\dot{\epsilon}_a$ | $1 \times 10^{-4} \text{s}^{-1}$ |
| Initial aging time                     | $t_0^a$            | 1 sec                            |
| <b>Initial conditions</b>              | <b>Notation</b>    | <b>Value</b>                     |
| Initial mobile dislocation density     | $\rho^m(0)$        | $1 \times 10^7 \text{m}^{-2}$    |
| Initial forest dislocation density     | $\rho^f(0)$        | $1 \times 10^{12} \text{m}^{-2}$ |

222 However, we conjecture that the DSA-endorsed plastic instabilities may be orientation de-  
223 pendent, and may therefore have significant or negligible impact on the overall mechanical  
224 response of the sample, depending on the crystal orientation. As a consequence, DSA-  
225 controlled nucleation, propagation, and intermittency of deformation bands might promote,  
226 leave unaffected, delay or impede crack propagation depending on the crystal orientation of  
227 the grain associated with the crack. Therefore, a study highlighting the influence of crystal  
228 orientation on DSA-triggered strain localization is now conducted.

229

230 To trigger the strain localization process, we introduce a sharp crack in the FE mesh (see  
231 Fig.3) by using the element dilution method where elements constituting the edge crack are  
232 assigned a negligible stiffness. A stiffness parameter  $K$  is used for this element degradation  
233 where the modified stiffness of the element is described as

$$\mathbf{C}_{mod} = (1 - K)\mathbf{C}, \quad (18)$$

234 where  $\mathbf{C}$  is the original elastic moduli tensor. Ideally, the parameter  $K$  for the elements  
235 shaping the edge crack should be 1. However, numerical stability puts a limit of  $K \approx 1$ ,  
236 whereas  $K$  is zero for the rest of the elements in the mesh. The single crystal with edge crack  
237 is discretized in  $50 \times 50 \times 10$  cubic elements (each cube being filled with tetrahedral elements)  
238 in the X, Y and Z directions. It is uniaxially loaded in  $y$  direction with fixed displacement  
239 rate, leading initially to mode-I type fracture stress concentration fields near the crack tip.  
240 This specifically serves as the source of early plastic strain localization and we do not con-  
241 sider any damage and crack propagation in this study. Frequently observed orientations,  
242 specific to rolled Al-Cu-Li-Mg alloys, (see Table 1) are chosen for this investigation. The  
243 Euler angles listed in Table 1 are taken from a previous work [31].

244

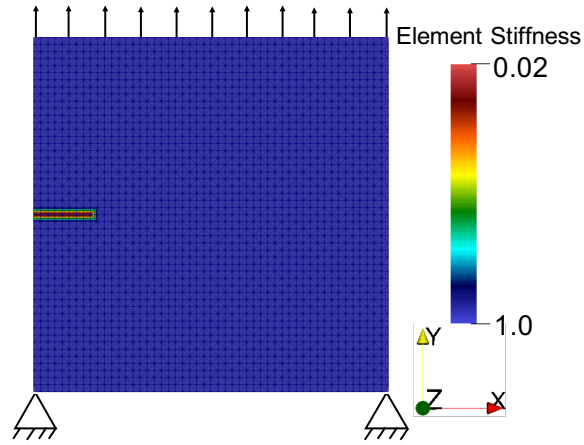


Figure 3: Single crystal with edge crack and uniaxial tension boundary condition used for FE simulations.

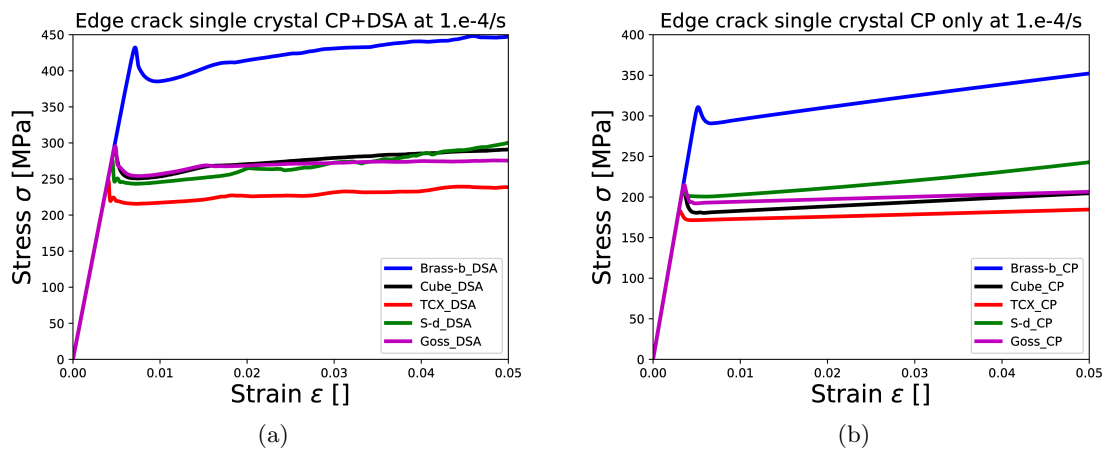


Figure 4: Orientation dependence of global deformation behavior of edge cracked single crystal loaded in fracture mode-I, (a) simulated with DSA-enabled crystal plasticity; (b) simulated with standard crystal plasticity (DSA absent).

245 As shown in Fig. 4, common to all crystal orientations and already observed in Fig. 2,  
 246 the average flow stress obtained from DSA-enabled CP is 50 to 100 MPa higher than from  
 247 the standard CP model (absent DSA). As already discussed, higher flow stress and larger  
 248 yield drop for the DSA-enabled CP model is the result of solute hardening and first solute-  
 249 dislocation breakaway event, respectively. As expected, the DSA-enabled model captures the  
 250 pinning and breakaway events manifested as stress serrations in the macroscopic stress strain  
 251 curve (see Fig. 4(a)), as compared to smooth flow stress curves obtained from the CP only  
 252 model in Fig. 4(b). Apart from the Brass-b orientation, which exhibits much higher strength,  
 253 all other orientations fall into a category of approximately comparable flow stresses. How-  
 254 ever, DSA alters the relative strength of the latter crystal orientations, if counterpart results  
 255 obtained from standard CP are taken as reference.  
 256

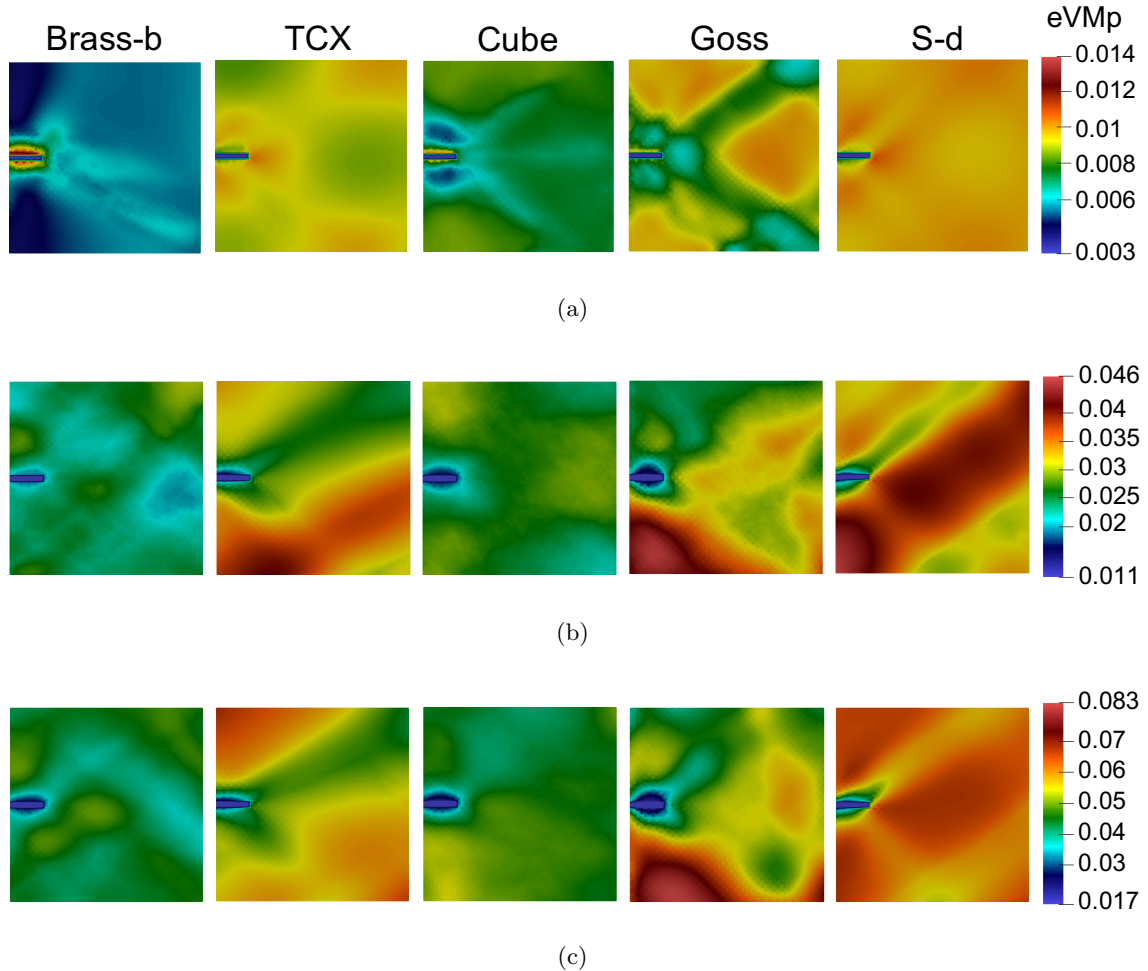


Figure 5: Equivalent von Mises plastic strain (eVMp) fields at gradually increasing global strains for different crystal orientations simulated using DSA-enabled CP model. The orientation dependence of DSA effects is manifested as divergent plastic zone extensions for the different crystal orientations under investigation, (a) eVMp at 1% global strain; (b) eVMp at 3% global strain; (c) eVMp at 5% global strain.

257 The influence of DSA is now examined at a local level in terms of the plastic strain  
 258 fields ahead of the crack tip and their evolutions with the applied overall strain, as compared  
 259 to standard CP predictions. The development of the plastic zones in the presence of DSA  
 260 (see Fig. 5) is observed to be less symmetric, more intense and more heterogeneous than for  
 261 the plastic zones obtained with standard CP shown in Fig. 6. The comparison also suggests  
 262 that DSA may be beneficial in delaying fracture nucleation and growth by shifting the strain  
 263 localization area away from the crack tip. In contrast, the absence of DSA results in strain lo-

264 calization right ahead of the crack tip, while producing more homogeneous strain fields away from the crack  
 265 from the crack. In addition, the above-mentioned influence of DSA is observed to be strongly  
 266 orientation dependent. Fig. 5 shows indeed a prominent crystal orientation dependence of  
 267 the DSA-triggered heterogeneous plastic zones (both ahead and away from the crack tip) at  
 268 gradually increasing global strain. A closer look at the plastic zones of individual orienta-  
 269 tions reveals that the Brass-b and Cubic orientations favor a relatively homogeneous plastic  
 270 strain field, whereas Goss, S-d and TCX promote a more localized plastic strain field within  
 271 the domain of simulation. Therefore, we may tentatively conclude that, while choosing the  
 272 crystal orientations to tailor a sample configuration less susceptible to strain localization in  
 273 the presence of DSA, the Brass-b and Cube orientations should be preferred over the S-d,  
 274 Goss and TCX orientations. In particular, the Brass-b orientation further exhibits a strong  
 275 increase of flow stress in the presence of DSA. However, forthcoming results for multilayered  
 276 crystal will show that such a conclusion is only provisional. In addition to the plastic strain  
 277 fields shown here, the reader may want to examine the nucleation, motion and intermittency  
 278 of the localized deformation bands by means of the equivalent strain rate fields provided as  
 279 videos in supplementary multimedia data. However, more details on the dynamics of strain  
 280 localization and the intermittency of dislocation activity will be provided in the next Section  
 281 (see Fig.11).

282

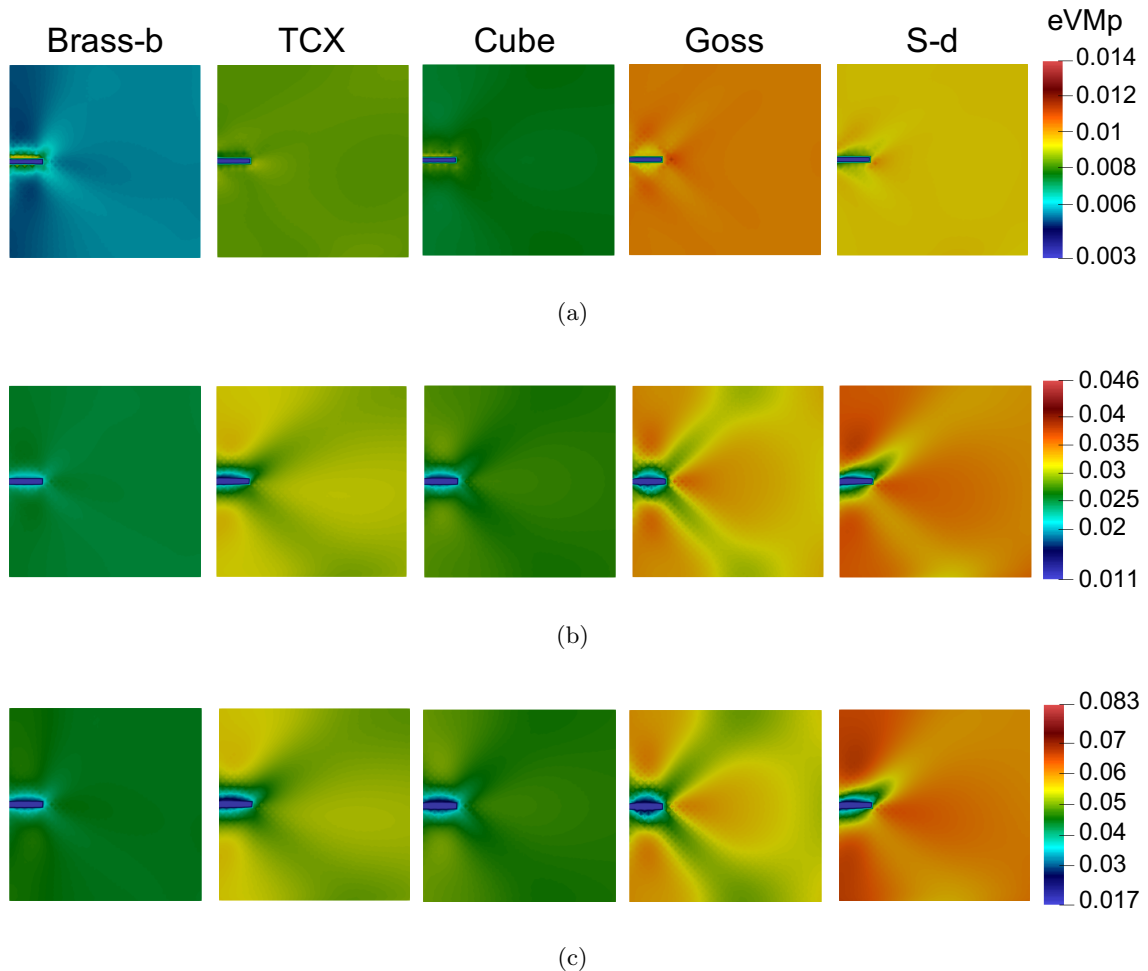


Figure 6: Equivalent von Mises plastic strain (eVMp) fields at gradually increasing global strains for different crystal orientations simulated with standard CP (DSA module absent), (a) eVMp at 1% global strain; (b) eVMp at 3% global strain; (c) eVMp at 5% global strain.

283 4.2. Edge cracked multi-layered polycrystal: effect of orientation couples

284 In the series of efforts made to generate a texture that is resistant to strain localization,  
 285 investigating the contribution of individual orientations is necessary but not sufficient. Grain  
 286 interactions may play a significant role, and the deformation behavior for a particular crystal  
 287 orientation may substantially differ from that obtained in the presence of neighboring grains  
 288 with different orientations. Therefore, we now conduct investigations using combinations of  
 289 orientation couples.

290

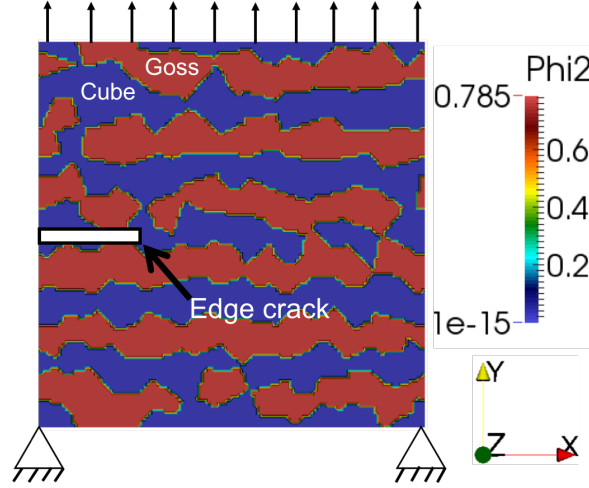


Figure 7: Edge-cracked multi-layered polycrystal with embedded orientation couples (here Cube-Goss) and uniaxial tension boundary conditions.

291 All of the  $C_2^5 = 10$  possible orientation couples obtained by considering the five frequently  
 292 observed orientations: Brass-b-Goss, Cube-TCX, Goss-S-d,..etc., were simulated in uniaxial  
 293 tension, both in presence and in absence of DSA. As before, the simulations performed with  
 294 the CP only model (without DSA) are used as references highlighting the influence of DSA  
 295 on the local fields and macroscopic stress-strain behavior. As shown in Fig. 7, a multi-layered  
 296 FE mesh inspired from the experimental observation of rolled microstructures of Al-Cu-Li-  
 297 Mg alloys is adopted to investigate the interaction of orientation couples.

298

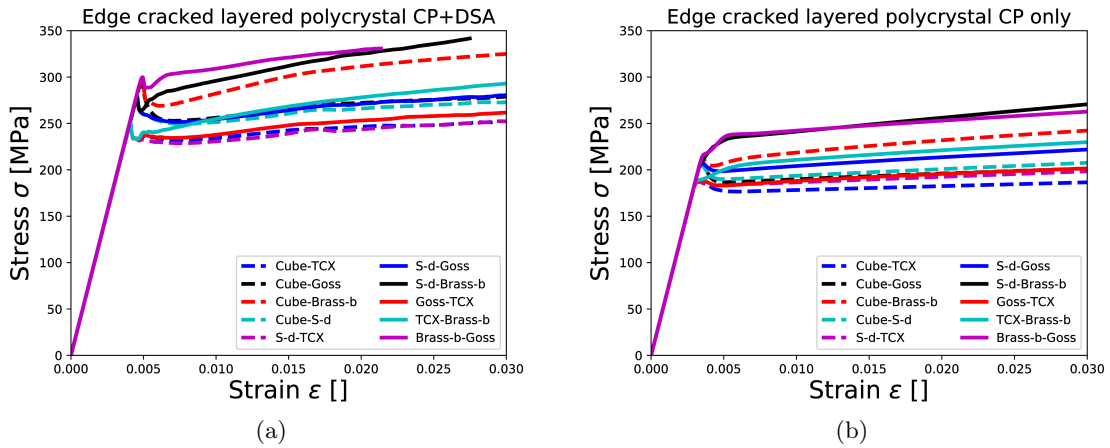


Figure 8: Averaged flow stress of edge cracked layered orientation couples loaded in fracture mode-I, (a) simulated with DSA enabled crystal plasticity; (b) simulated with standard crystal plasticity (DSA absent).

299 Similar to single crystal results, the layered polycrystalline morphology exhibits promi-  
 300 nent differences in the macroscopic stress-strain curves obtained from the DSA-enabled CP  
 301 model as compared to standard CP calculations (see Fig. 8). As already found, higher flow  
 302 stresses and larger yield drops obtained for the DSA-enabled model can be associated with  
 303 the solute stress and first solute-dislocation breakaway event, respectively. The macroscopic  
 304 stress-strain curves obtained from DSA-enabled CP can be relatively divided in two cat-  
 305 egories: orientation couples containing Brass-b and others excluding Brass-b. Indeed, it is  
 306 observed that coupling any orientation with the Brass-b orientation results in a 50 to 100 MPa  
 307 boost in the macroscopic flow stress, with the notable exception of TCX–Brass-b. The in-  
 308 fluence of DSA is also evident from small but crucial changes in the relative flow stresses for  
 309 different orientation couples as compared to results obtained using standard CP.  
 310

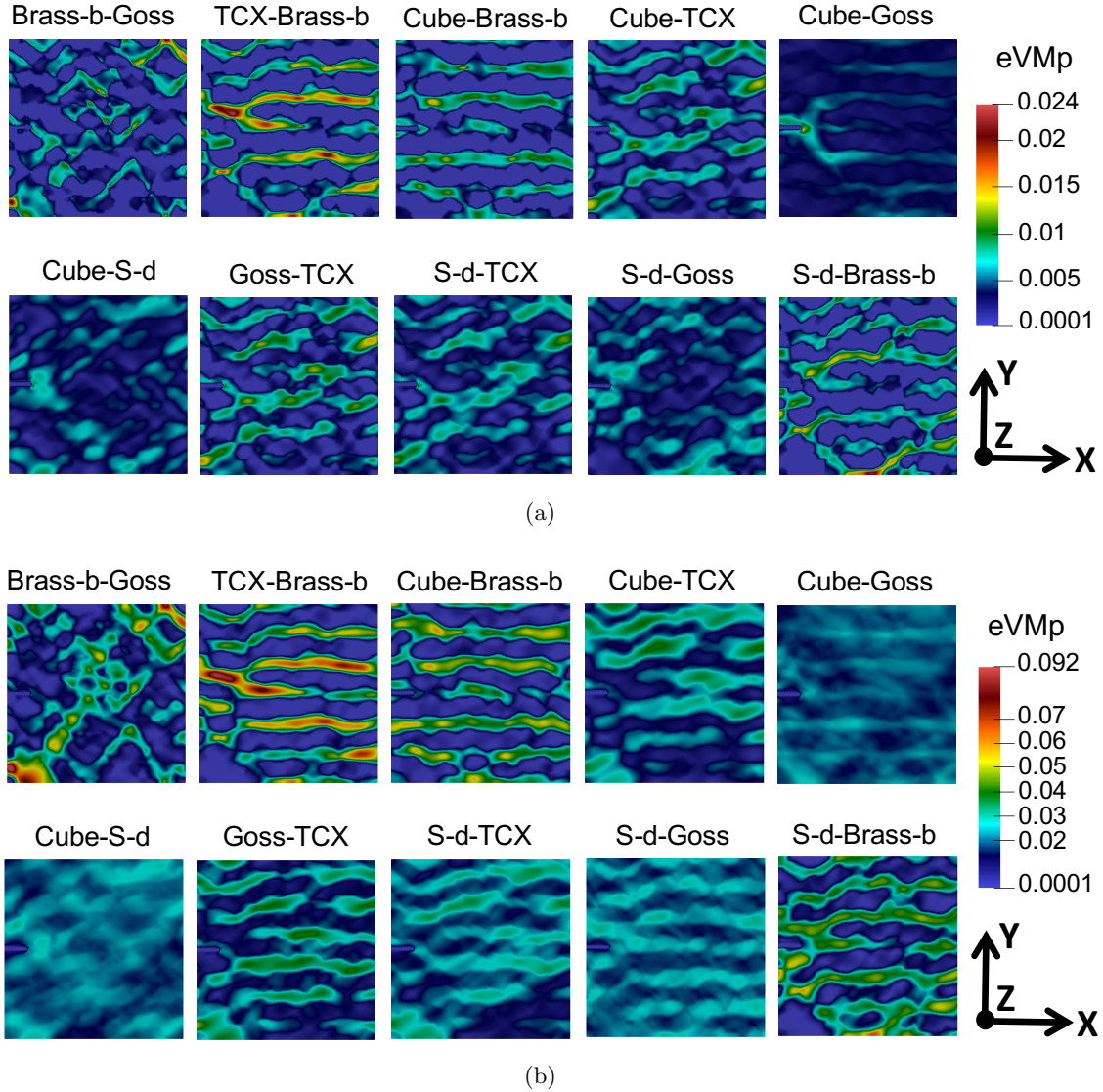


Figure 9: Equivalent plastic strain (eVMp) fields at gradually increasing global strains for different orientation couples. DSA plays a significant role in changing the behavior of a particular orientation in the presence of other crystal orientations, (a) eVMp at 0.6% global strain; (b) eVMp at 2% global strain.

311 The analysis of the predicted plastic strain fields is now conducted to investigate the  
 312 joint influences of grain orientation couples and DSA on strain localization leading to failure.  
 313 To this end, Fig. 9 presents the equivalent plastic strain (eVMp) fields predicted for the ten  
 314 orientation couples at two distinct strain levels: 0.6%, which is close to the elasto-plastic

315 transition, and 2%, that is in the hardening regime. For most of the orientation couples,  
316 the initiation of the plastic zone swiftly migrates away from the crack tip in the presence of  
317 DSA, which may have again a stabilizing influence on incoming crack propagation, and the  
318 high strain zones are found to be rather independent of the edge crack location. The plastic  
319 strain fields for the various orientation couples can be broadly divided into two categories:  
320 orientation couples exhibiting highly heterogeneous strain distributions, and orientation cou-  
321 ples displaying rather homogeneous strain distributions (see Fig. 9(b)). Most notably and  
322 in strong contrast with the beneficial properties of the Brass-b orientation for single crys-  
323 tal simulations, nearly all the orientations coupled with Brass-b now demonstrate strong  
324 strain localization and heterogeneous plastic strain fields as compared to other couplings, a  
325 property that can be detrimental with respect to strain localization leading to fracture. In  
326 particular, TCX–Brass-b shows the strongest strain localization trend, which can be related  
327 to its relatively low hardening rate in Fig. 8. Such a result highlights the importance of con-  
328 sidering the effects of grain neighborhood and grain-to-grain interactions. On the contrary,  
329 mutual couplings of S-d, Goss and Cube orientations promote a rather homogeneous plastic  
330 strain distribution, and therefore could well be better candidates while choosing orientation  
331 distributions less prone to strain localization. Note that the simulations predict a strong  
332 anisotropy of plastic deformation in grains, with possible high contrast between grains, in  
333 particular for Brass-b/S-d couples, which is in good agreement with available experimental  
334 and modeling data [32–34].

335

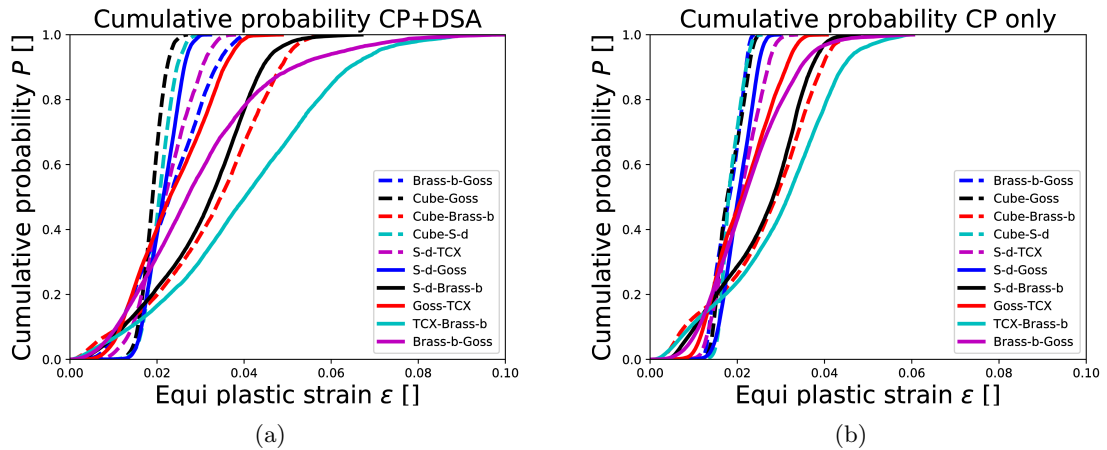


Figure 10: Cumulative probability distributions of the equivalent plastic strain at 0.02 average tensile strain for edge cracked layered orientation couples loaded in fracture mode-I, (a) simulated with DSA-enabled CP; (b) simulated with standard CP (DSA absent).

336 A more synthetic presentation of the above-discussed strong vs. weak strain localization  
337 patterns pertaining to different orientation couples is shown in Fig. 10 where the cumulative  
338 probability of equivalent plastic strain (eVMp) is computed and plotted at 2% global strain  
339 for all orientation couples. To interpret these plots, note that a narrow cumulative probability  
340 of plastic strain suggests a small scatter of plastic strain throughout the sample, and hence a  
341 rather homogeneous plastic strain field. As compared to standard CP results, a larger spread  
342 in the cumulative probability obtained from DSA-enabled CP is a direct indication of DSA  
343 triggered stronger heterogeneity in eVMp (see Fig. 10(a) and 10(b)). In addition, the cumu-  
344 lative probability spread is found to be larger in the presence of the Brass-b orientation, as  
345 compared to mutual couplings of the S-d, Goss and Cube orientations, which again points to  
346 a stronger strain heterogeneity. In particular, the TCX–Brass-b orientation couple exhibits  
347 the larger spread and higher strain heterogeneity, with local strains nearly reaching 0.1 at a  
348 macroscopic strain of 0.02.



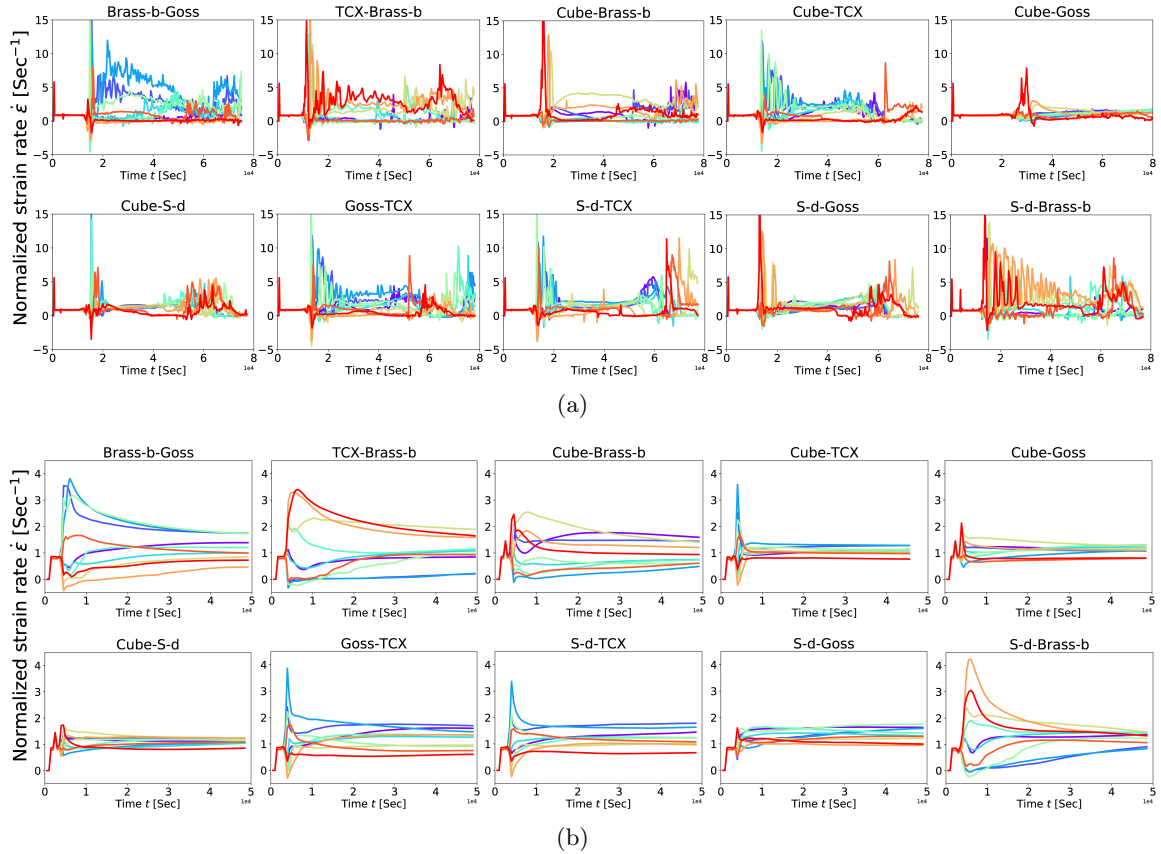


Figure 11: Time evolution of strain rate for randomly chosen nodes in the mesh, (a) simulated with DSA enabled crystal plasticity; (b) simulated with standard crystal plasticity (DSA absent).

350 Finally, the intermittency of the equivalent strain rate field  $\dot{\epsilon}_{eq}$  is examined in relation with  
 351 its heterogeneity by plotting this quantity in Fig. 11, normalized by the overall applied strain  
 352 rate  $\dot{\epsilon}_a$ , at ten different (randomly chosen) locations in the sample. In comparison to smooth  
 353 strain rate variations obtained from standard CP and shown in Fig. 11(b), DSA-enabled CP  
 354 clearly yields a recurrence of sharp peaks, *i.e.* a highly intermittent behavior often associated  
 355 with the PLC effect (Fig. 11(a)). Further, the heterogeneity apparent in Fig. 11(b), which  
 356 simply derives from location and orientation differences, is found to be amplified by DSA in  
 357 Fig. 11(a), and intermittency usually appears to be highest at locations where the equivalent  
 358 strain rate is the largest. Of course, the calculations shown in Fig. 11 confirm that the  
 359 intermittency observed in the DSA-enabled CP simulations is a direct consequence of the  
 360 dislocation-solute interactions, by which every peak in the strain rate spatiotemporal field is  
 361 associated with a particular set of pinning and breakaway events.

## 362 5. Conclusions

363 The primary findings of the presented investigation can be summarized as follows:

- 364 1. A successful slip system-based implementation of a DSA constitutive model, coupling  
 365 the dynamics of mobile and sessile dislocation densities in standard small scale crystal  
 366 plasticity, allows accurately mimicking the experimental observations for dilute Al-Cu-  
 367 Li-Mg alloys. We are able to capture both macroscopic serrated stress-strain curves  
 368 and plastic strain and strain rate fields involving recurrent nucleation and propagation  
 369 of strain localization bands on various slip systems, as observed in experiments. In  
 370 contrast, a smooth flow stress and complete absence of plastic instabilities is seen for  
 371 the standard CP model (DSA module absent).

- 372 2. Simulations of edge cracked single crystals loaded in fracture mode-I demonstrated a  
373 strong orientation dependence of the destabilizing effects of DSA. The development of  
374 a plastic strain localization area is observed to be quite localized for orientations such  
375 as Goss, S-d and TCX, whereas the Brass-b and Cube orientations favor a relatively  
376 homogeneous plastic strain field.
- 377 3. The results obtained from investigating orientation couples highlight the strong influ-  
378 ence of the latter on the destabilizing effects of DSA. Nearly all the orientations in the  
379 presence of Brass-b demonstrate stronger strain localization patterns and more hetero-  
380 geneous plastic strain fields than the mutual couplings of S-d, Goss and Cube. The  
381 latter are therefore found to be beneficial in terms of homogeneous strain distribution.  
382 The rather opposite influences of the Brass-b orientation, paradoxically seen as a sta-  
383 bilizing factor in single crystal simulations and a destabilizing one when neighboring  
384 grains are taken into account, highlight the importance of grain neighborhood as well  
385 as grain-to-grain interactions in microstructures.

386 It is important to note that above mentioned outcomes are true for solicitation in the trans-  
387 verse directions and propagation in the rolling direction. We expect a significant changes  
388 in conclusion for traction in the rolling direction and propagation in the transverse direc-  
389 tion, which could be a potential outlook for the present work. Further steps in this research  
390 involve the simulation of a more realistic Kahn tear test with a sample containing a large  
391 number of grains, such as to investigate in more details the role of texture and grain-to-grain  
392 interactions in the early localization phenomena. To this end, a numerical spectral method  
393 using Fast Fourier transforms (FFT) algorithms [42, 43] will be considered. Spectral CP-FFT  
394 methods are computationally much more efficient than the CP-FEA methods, which allows  
395 dealing with much larger polycrystalline samples, with foreseeable benefits in the prediction  
396 of textures at large strains. The only inherent rigidity attached to spectral methods, i.e.  
397 need of periodic boundary conditions can be averted by using buffer zones at the sample  
398 boundaries. Further, in AA-2198-T8 alloys, the beneficial role of nanosize T1 precipitates  
399 in terms of strength and strain homogenization will be investigated [16–19]. It was recently  
400 demonstrated that certainly such platelet precipitates, which form mostly on dislocation lines  
401 on  $\{111\}$  slip planes during an artificial heat treatment applied to T3 alloys, have a hetero-  
402 geneous spatial distribution and cannot be sheared twice by dislocation lines at the same  
403 location, which limits dislocation avalanches. While early strain localization is still observed  
404 in the Kahn tear tests of AA-2198-T8 alloys [13], the competition between T1 precipitates  
405 and dynamic strain aging on strain localization is thought to be important and a constitutive  
406 law accounting for precipitates will be developed, which will allow refining microstructure  
407 design in view of limiting strain localization phenomena.

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413

## 414 Declaration of interest

415 None

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