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# Three dimensional simulations of texture and triaxiality effects on the plasticity of magnesium alloys

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ABSTRACT

We investigate the synergistic effects of texture and intrinsic plastic anisotropy (at the level of single crystal) on the deformation of polycrystalline magnesium using three-dimensional crystal plasticity finite element simulations. Using rolled plate texture as a basis, we simulate the deformation using a range of synthetic textures. Smooth and notched round bar specimens are considered to achieve different levels of stress triaxiality. Two sets of constituent single crystal properties, representative of an Mg alloy and pure Mg respectively, are adopted in order to investigate the role of intrinsic plastic anisotropy. Our results reveal that textural variations couple into the intrinsic plastic anisotropy and triaxiality to determine the active deformation mechanisms. When loaded along the rolling direction of the plate, the deformation is accommodated by prismatic slip at low triaxiality and pyramidal $\langle c+a \rangle$ slip at high triaxiality. Softer mechanisms such as basal slip and extension twinning, which are not favored by the loading orientation, are activated due to the intergranular stresses. The smooth specimens show macroscopic strain localization the onset of which depends on initial texture. The deformed textures are strongly modulated by both triaxiality and intrinsic plastic anisotropy. We also briefly discuss the potential role of twinning in damage evolution.



## 1. Introduction

Microstructure, material properties and macroscopic stress state closely interact in determining the strength and fracture resistance of ductile metals. While a fair understanding of the nexus between microstructure and stress state on damage evolution has been achieved through experiments and modeling for common engineering metal alloys, the same is not true for low crystal symmetry materials [1]. In HCP metals, for instance, textural effects couple into intrinsic (single crystal) plastic anisotropy, having significant ramifications on their macroscopic characteristics. This behavior has been well documented through experiments and modeling under uniaxial and biaxial (plane stress and plane strain) states [2–5]. However, a definitive assessment of the role of stress state and its relationship with texture, intrinsic plastic anisotropy and deformation mechanisms is not yet established; such an assessment is particularly important because of their implications on failure mechanisms [6–8]. In this work, we take a step towards understanding the connections between stress triaxiality, texture and intrinsic plastic anisotropy in magnesium (Mg) and Mg alloys, which have seen a resurgence as structural materials.

Experimental works that systematically investigate the role of stress state in Mg are beginning to emerge with an obvious interest in its effect on damage. Three-point bend tests on notched single crystal Mg suggested a positive correlation between the energy release rate and $\{10\bar{1}2\}$ extension twin fraction [9]. Prasad et al. [10] observed significant extension twinning ahead of the notch root despite an unfavorable texture in their compact tension experiments on Mg alloy AZ31B with rolled texture. Contrasting observations on the nature of damage mechanisms, micro-void sheeting [11] versus micro-void growth and coalescence [10], have been reported. Kondori and Benzerga [12] investigated stress state effects on fracture of rolled polycrystalline AZ31B alloy using round uniform and notched specimens. They reported several salient features, not commonly observed in ductile metals - round uniaxial tension specimens exhibited shear failure; with increasing stress triaxiality, the

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**Table 1**
Slip and twin systems considered in this work.

| | Slip/twin plane | Slip/twin direction | Number of systems |
|---|---|---|---|
| Basal Slip | $(0001)$ | $\langle 11\bar{2}0\rangle$ | 3 |
| Prismatic $\langle a\rangle$ Slip | $\{10\bar{1}0\}$ | $\langle 11\bar{2}0\rangle$ | 3 |
| Pyramidal $\langle a\rangle$ Slip | $\{10\bar{1}1\}$ | $\langle 11\bar{2}0\rangle$ | 6 |
| Pyramidal $\langle c+a\rangle$ Slip | $\{11\bar{2}2\}$ | $\langle 11\bar{2}3\rangle$ | 6 |
| Extension Twinning (ET) | $\{10\bar{1}2\}$ | $\langle 10\bar{1}1\rangle$ | 6 |
| Contraction Twinning (CT) | $\{10\bar{1}1\}$ | $\langle 10\bar{1}2\rangle$ | 6 |

fracture strains showed a non-monotonic dependence on stress triaxiality with peak ductility occurring at intermediate nominal triaxiality. While void growth and coalescence were observed corresponding to peak ductility, at higher stress triaxiality, quasi-brittle type fracture surfaces were evident concomitant with lower ductility. The role of alloy composition (which affects the plastic anisotropy) has also been studied. Round notch bar experiments on a magnesium-rare earth alloy (WE43) with a weaker rolled texture indicated that, although the fracture strain showed a qualitatively similar trend with notch acuity as in the AZ31B alloy, the notch ductility was much lower in WE43 [7]. This hints at more complex interactions between texture and failure mechanisms than currently appreciated. Furthermore, both uniform and round notch bar specimens showed no significant evidence of void growth mechanisms; instead, fracture surfaces indicated intergranular cracking, cleavage and ductile tearing. Even more recently, Ray and Wilkinson [8] compared the fracture behavior of flat tapered tensile specimens of another Mg rare-earth alloy (ZEK100) with AZ31B alloy; though the final failure involved a macroscopic shear localization in both alloys, ZEK100 exhibited a quasi-brittle fracture surface with linkage of twin induced microcracks whereas AZ31B showed quasi-ductile fracture surface involving void linkage.

Very recently, we investigated the interplay between the stress triaxiality and intrinsic plastic anisotropy in Mg that revealed complex characteristics of the macroscopic deformation anisotropy and their micromechanical underpinnings in notched specimens [13]; the work indicated the important role of intrinsic plastic anisotropy in the deformation of Mg. However the analysis of Selvarajou et al. [13] was limited to single crystals. This work aims at providing fundamental insights into effects of texture on the plasticity of Mg and its alloys through three-dimensional crystal plasticity based finite element simulations. Our approach here is to use simulated rolling textures with systematically varying degrees of in-plane and out-of-plane textural deviations and incorporating them into idealized polycrystalline specimens. The effect of stress triaxiality is studied by considering smooth and notched round bars of different notch acuities. Further, for each initial texture two sets of single crystal material parameters, one representative of an Mg alloy and the other corresponding to pure Mg are adopted in order to highlight separately the role of texture and that of intrinsic (single-crystal level) plastic anisotropy.

## 2. Computational framework

The HCP crystal plasticity model (HCP-CP) developed by Zhang and Joshi [14] and implemented as a User MATerial (UMAT) subroutine in ABAQUS/STANDARD® [15] is adopted as the constitutive framework. It considers eighteen slip and twelve twin systems (Table 1). A brief description of the formulation is given in Appendix A.

### 2.1. Simulation set-up

Fig. 1a–c depicts typical meshes used in the calculations for the smooth and notched specimens, which conform to the experiments of Kondori and Benzerga [12]. The round notched specimens are identified as RN$\xi$ with $\xi = 10\mathrm{R}/D_0$ where R is the notch radius. The plate's transverse ($T$), rolling ($L$) and normal ($S$) directions are aligned with the global X, Y and Z axes, respectively. A baseline mesh (Mesh-1) and two finer meshes (Mesh-2 and Mesh-3) are created which are respectively discretized into ~ 23,000, ~ 35,000 and ~ 80,000 eight-node hexahedral elements with reduced integration. Fig. 1d shows the cross section of the three meshes of the smooth specimen; similar refined meshes are created for other specimen geometries as well. All specimens are loaded in tension along $T$ (the global Y axis) with a constant displacement rate $\dot{U}$ applied at the top surface of the specimen keeping the bottom surface fixed along Y; sufficient constraints to suppress rigid body motion are imposed. The nominal strain rate $\bar{\dot{\varepsilon}} = \dot{U}/L_0 = 1 \times 10^{-3}\ \mathrm{s}^{-1}$, where $L_0$ is the length of the specimen, is maintained. Since the input displacement rate in all specimens is the same, the axial strain rate in the notch region is specimen dependent. However, the low strain rate sensitivity parameter adopted in this work ($m = 50$ for all slip and twin systems) ensures that the results are not influenced by the variations in local strain rates. We verified this by performing a calculation for the RN2 specimen at a nominal strain rate of $1 \times 10^{-3}\ \mathrm{s}^{-1}$ calculated based on the notch height rather than the specimen length.

### 2.2. Polycrystal model

A polycrystal is created by post processing the finite element mesh as follows: for a given specimen, a grain is defined by grouping a fixed number of elements and assigning a unique crystallographic orientation to that element group. For the smooth specimen, the entire volume is divided into several grains whereas for the notched specimens, only the notch volume is considered for the polycrystalline representation while the remaining region is assigned a fixed single crystal orientation. This is reasonable because, our previous work [13] shows that in notched specimens, the deformation processes are restricted to the notch region. We ensure that the grain junctions formed are triple junctions (as opposed to quadruple junctions typically used in polycrystalline simulations) to obtain realistic intergranular interactions. The number of elements that constitute a grain is different for different specimens; however, the total number of grains $N_g$ in each specimen is kept approximately the same so that a systematic comparison can be made for a family of smooth and notched specimens with the same initial texture (Table 2).

### 2.3. Texture generation

Every grain has a crystallographic label, an Euler angle set $\{E\} = \{\varphi_1, \Phi, \varphi_2\}$, comprising the Euler rotation angles associated with that grain. As an independent single crystal, an individual grain initially has its $[10\bar{1}0]$ and $[0001]$ directions aligned with the global X and Z directions, respectively. Then, an Euler rotation is applied to the grain by following the Bunge rotation scheme. Table 3 summarizes the effect of each of the three Euler angles in determining the actual orientation of a grain in a polycrystal with respect to the sheet directions. For a polycrystalline sample with $N_g$ grains, the required $N_g$ Euler angle sets are generated as follows: for each of the three angles in $\{E\} = \{\varphi_1, \Phi, \varphi_2\}$, normal distributions of $N_g$ angles each with mean value equal to zero and standard deviation $\{\Delta E\} = \{\Delta\varphi_1, \Delta\Phi, \Delta\varphi_2\}$ respectively are generated. From the three distributions, an Euler angle set is formed by randomly