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On plastic flow in notched hexagonal close packed single crystals

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ABSTRACT

The micromechanics of anisotropic plastic flow by combined slip and twinning is investigated computationally in single crystal notched specimens. Constitutive relations for hexagonal close packed materials are used which take into account elastic anisotropy, thirty potential deformation systems, various hardening mechanisms and rate-sensitivity. The specimens are loaded perpendicular to the *c*-axis but the presence of a notch generates three-dimensional triaxial stress states. The study is motivated by recent experiments on a polycrystalline magnesium alloy. To enable comparisons with these where appropriate, three sets of activation thresholds for the various deformation systems are used. For the conditions that most closely mimic the alloy material, attention is focused on the relative roles of pyramidal $\langle c+a \rangle$ and prismatic $\langle a \rangle$ slip, as well as on the emergence of $\{10\bar{1}2\}[10\bar{1}1]$ extension twinning at sufficiently high triaxiality. In all cases, the spatial variations of stress triaxiality and plastic strain, inclusive of various system activities, are quantified along with their evolution upon straining. The implications of these findings in fundamental understanding of ductile failure of HCP alloys in general and Mg alloys in particular are discussed.

1. Introduction

In materials with high crystal structure symmetry, e.g. FCC metals, plastic flow mainly occurs via dislocation mediated slip. There, the critical resolved shear stresses (CRSS) for activating different slip systems are nearly the same (Asaro and Needleman, 1985). This renders weakly anisotropic plasticity at the single crystal level. In such materials, plastic flow anisotropy may occur due to texture or grain elongation arising, for example, from severe pre-deformation during processing (Asaro and Needleman, 1985; Wenk and Van Houtte, 2004). A more fundamental origin of plastic anisotropy arises from disparate activation thresholds for various deformation mechanisms, a situation which is typical of materials with low crystal symmetry. We refer to this as *inherent plastic anisotropy* – the ratio of the CRSS of a slip/twin system relative to another slip/twin system. An example of this kind are materials with hexagonal close packed (HCP) crystal structure, which can deform by slip and twinning (Christian and Mahajan, 1995). In pure magnesium (Mg) the CRSS ratio of the hardest to softest slip modes is of order 100 (Kelley, 1967; Chapuis and Driver, 2011). Due to the low symmetry of the crystal structure, this type of anisotropy couples into polycrystalline texture effects.

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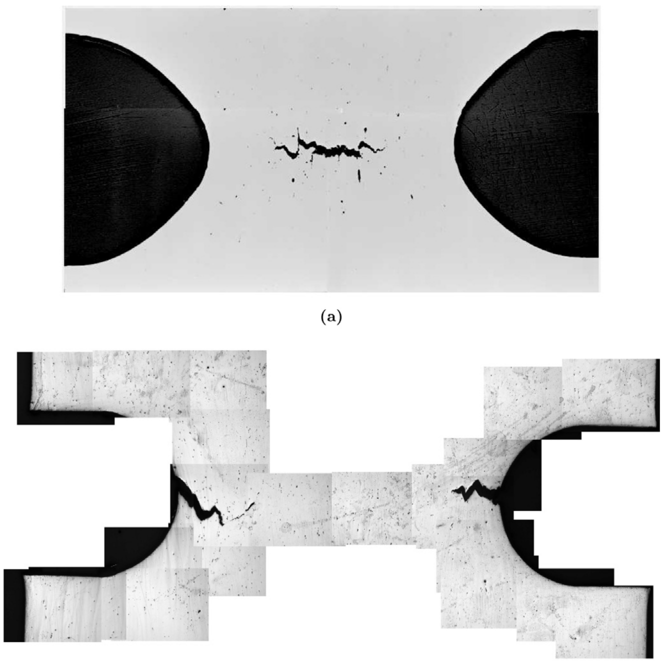
The strong anisotropy of HCP metals such as Mg is often referred to as the origin of their damage intolerance (Bohlen et al., 2007), although it has not prevented some other HCP metal alloys, such as Zr- or Ti-based alloys, from being used as structural materials. There is a fair amount of research on characterizing plastic anisotropy in HCP metals in relation with fundamental deformation mechanisms: Ti (Wu et al., 2008), Zr (Lebensohn and Tomé, 1993), Mg (Staroselsky and Anand, 2003; Agnew and Duygulu, 2005), among many others. Most studies focus, however, on uniaxial loading conditions. On the other hand, the influence of plastic anisotropy on failure under multiaxial stress states is not well understood. While this is generally relevant to textured polycrystals of high-symmetry materials, it is particularly important for low-symmetry materials. From considerations of failure micromechanics, the three-dimensional character of stress state at the current material point can be quantified by the stress triaxiality ratio, henceforth referred to simply as triaxiality, $\mathsf{T} = \sigma_h/\sigma_e$ where σ_h is the hydrostatic stress and σ_e is the von Mises equivalent stress. In metals, positive (tensile) triaxiality has implications on the nucleation and evolution of voids (Gurson, 1977; Benzerga and Leblond, 2010; Pineau et al., 2016). A common experimental approach to investigating triaxiality effects is to adopt notched specimens where various triaxiality levels can be generated by choosing appropriate notch geometries (Hancock and MacKenzie, 1976; Pineau et al., 2016). While smooth round bar specimens result in a constant $\mathsf{T} = 1/3$ (before necking), those with circular notches can produce $0.5 \lesssim \mathsf{T} \lesssim 1.5$ depending on the notch root radius (Needleman and Tvergaard, 1984).

An important consideration in the ductile fracture of any metallic alloy is the interplay between plastic strain and triaxiality. In particular, notched bars are ideal specimens to investigate such competition (Needleman and Tvergaard, 1984). In round notched bars, the plastic strain is usually maximum at the notch root, particularly in the early stages of straining. By way of contrast, the maximum triaxiality moves to the center of the bar after a short transient. In ductile metals a macroscopic crack typically initiates at the center of the bar, indicating a strong triaxiality effect (Hancock and MacKenzie, 1976; Needleman and Tvergaard, 1984; Hancock and Brown, 1983). Fig. 1a illustrates this situation for steel. In less ductile metals, the macroscopic crack initiates close to but away from the notch root, then eventually links to the surface in the form of a shear crack (in certain planes). This situation applies to Mg alloy AZ31, as shown in Fig. 1b. While this observation indicates that crack initiation in less ductile metals is driven by plastic strain concentrations (Alves and Jones, 1999), a mediating effect of triaxiality is not excluded. What is of particular importance, therefore, is that a fine description of plasticity in these materials is needed to develop a consistent theory of damage accumulation to fracture.

Anisotropic models coupling plasticity and damage by way of homogenization have been developed with increasing levels of sophistication (Benzerga and Leblond, 2010; Benzerga et al., 2016). In these models, anisotropic plasticity is typically represented using quadratic yield criteria (Benzerga and Besson, 2001; Keralavarma and Benzerga, 2008; Monchiet et al., 2008) or relatively simple accounts of tension–compression asymmetry (Stewart and Cazacu, 2011). Applications of such models to engineering materials remain scarce, even for high-symmetry materials, e.g. Benzerga et al. (2004a,b) and Tanguy et al. (2008). In the above applications, the net anisotropy in fracture is often traceable to void shape and spatial distribution effects. On the sole basis of experiments, it is unclear to what extent the plastic anisotropy of the matrix itself



(a)

(b)

Fig. 1. Comparison between the outline and location of macroscopic cracks in (a) a low carbon medium alloy steel (Benzerga, 2000) and (b) AZ31 magnesium alloy (Kondori, 2015).