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Nature of crack-tip plastic zone in metallic glasses

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The fracture of metallic glasses(MGs) can be induced by shear banding in a ductile mode or by cavitation in a brittle way. Plastic zone in front of a crack tip, which is greatly involved with localized shear band, cavitation and the resultant fracture morphology, is a key clue to unveil the secrets of the intrinsic ductility and fracture. However, the characteristics of plastic zone, i.e., stress and strain distributions, size and shape, have not been clearly unraveled for MGs so far. In this paper, an analytical solution of the plastic zone for mode I crack under plane strain condition is derived through *J*-integral based on a slip line field analysis and shape approximation, by taking pressure-sensitivity, dilatancy, and structural evolution into account. Two length scales of the plastic zone, i.e. the maximum radius R_{max} and the radius along the crack line direction R_x, are revealed to control shear flow instability and cavitation, and therefore failure modes. According to shear transformation zone (STZ) based free volume evolution dynamics, the critical values of the mode I stress intensity factor and the plastic zone size at crack initiation are obtained. The effects of Poisson's ratio, pressure sensitivity, and dilatancy on the stress/strain distributions, and the size of plastic zone are elucidated. It is found that larger Poisson's ratio and smaller dilatancy lead to higher fracture toughness and 'slender' critical plastic zone, facilitating a good ductility. The internal correlations of the fracture pattern (i.e. dimple structure) with the plastic zone are established, where the size of the fracture pattern is quantitatively characterized by the critical length of plastic zone. To be further, a shape change of the critical plastic zone from 'slender' (apt to shear plastic flow) to 'chubby' (inclined to cavitation) is revealed with increasing dilatancy or decreasing Poisson's ratio, which might shed light on the underlying mechanism of ductile-to-brittle transition in MGs.

1. Introduction

Compared with crystalline order, more materials in nature prefer to exist in a disordered state, e.g. noncrystalline/amorphous solids and granular materials. Due to the absence of long-range structural order, plastic deformation in disordered solids is not accommodated by dislocation but through localized shear-driven rearrangements involving a small number of so-called plastic units (clusters of atoms/molecules/grains) (Spaepen, 1977; Argon, 1979; Falk and Langer, 1998). Some fundamental and unique mechanical traits are found in these materials (Rudnicki and Rice, 1975; Li and Pan, 1990a,b; Flores and Dauskardt, 2001; Schuh et al., 2007), such as the considerable pressure sensitivity in yielding, shear dilatancy during the

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deformation, and more complex failure behavior in contrast to that of ordered ones. The mysteries within the disordered materials arouse great interests of researchers but there still lots of problems remain elusive (Miracle, 2004; Falk and Langer, 2011; Biroli, 2014; Goodrich et al., 2014; Kamrin and Bouchbinder, 2014). As a new member of disordered materials, metallic glasses (MGs) behave as a double-blade sword for their extremely high strengths but poor room-temperature ductility. Their intrinsic inability to undergo finite plastic straining under tension greatly impedes MGs from wide structural usage. The underlying deformation and fracture physics, being one of the most fundamental problems of MGs, has attracted substantial research effort for the last decades (Spaepen, 1975; Argon and Salama, 1976; Ravichandran and Molinari, 2005; Schuh et al., 2007; Jiang et al., 2008a; Raghavan et al., 2009; Tandaiya et al., 2009; Xu et al., 2010; Chen et al., 2011; Jang et al., 2011; Greer et al., 2013; Tandaiya et al., 2013; Narayan et al., 2014; Narasimhan et al., 2015). Due to their special atomic structures, MGs may go through ductile failure via shear banding (Dai et al., 2005; Jiang et al., 2008b; Chen and Lin, 2010; Chen et al., 2013; Greer et al., 2013) or brittle fracture by cavitation (Jiang et al., 2008a; Murali et al., 2011a; Singh et al., 2013, 2014). At nanoscale, these inelastic deformation and fracture is accommodated by atomic clusters called as shear transformation zones (STZs) (Argon, 1979; Falk and Langer, 1998) or tension transformation zones (TTZs) (Jiang et al., 2008a; Huang et al., 2014a). The initiation and propagation of a shear band or a crack largely depend on the surrounding stress and deformation fields (Tandaiya et al., 2007, 2008; Huang et al., 2014b; Wu et al., 2015). As a critical region ahead of the crack tip, plastic zone may trigger or inhibit the shear banding or cracking and therefore determine the overall deformation and failure behavior, being a bridge between the micro-deformation and the macro-failure (Ashby and Greer, 2006).

From the viewpoint of phenomenological fracture mechanics, the ductile or brittle fracture through the initiation and growth of a crack depends on the surrounding stress and deformation fields near the tip. A number of important works have been made on the stress and strain fields ahead of the crack tip for ideally-plastic and power-law hardening materials. The *J*-integral for plane cracks is widely exploited for studying fracture in both linear and non-linear elastic materials, through which a approximate solution of plastic zone for ideally-plastic material was concluded combined with the slip line field analysis (Rice, 1968). Pan and Shih (1986, 1988) obtained the crack-tip fields for power-law hardening orthotropic materials. These fields are of the Hutchinson-Rice-Rosengren (HRR) type, and the deformations of these fields are volume preserving. An example of the HRR type crack-tip fields with volumetric deformation was presented by Hutchinson (1983) for power-law creep materials undergoing creep-constrained grain boundary cavitation. As for pressure-sensitive dilatant materials, Li and Pan (1990a,b) analyzed the crack-tip stress and strain fields under 2D plane stress and strain conditions, by introducing a hydrostatic stress-dependent yield criterion and the normality flow rule. They also obtained mode I crack-tip fields for power-law hardening materials within a limited degree of pressure sensitivity. Based on the Drucker–Prager yield criterion, Jeong et al. (1994) constructed theoretical slip lines in front of a round notch tip in a pressure sensitive material. Basu and Van der Giessen (2002) conducted a finite deformation analysis of crack tip fields in glassy polymers using a viscoplastic constitutive model that incorporated softening as well as orientation hardening. For pressure sensitive plastic solids, Subramanya et al. (2007) performed a 3D finite element analysis of mode I crack tip fields under small-scale yielding (SSY) conditions. The crack tip for MGs was studied by Tandaiya et al.(2007, 2008), by using a continuum elastic-viscoplastic constitutive theory developed by Anand and Su (2005), and it was found that these features of plastic field, in turn, are influenced by the mechanical characteristics of MGs like Poisson's ratio and pressure sensitivity. Henann and Anand (2009) conducted finite-element simulations of fracture initiation at notch tip in a MG under mode I, plain-strain, SSY conditions, and revealed the correlations of the fracture toughness with notch-tip radius and elastic modulus. Combining a simple version of the STZ model with an advanced Eulerian level set formulation, Rycroft and Bouchbinder (2012) analyzed the crack tip behavior of a blunted straight notch under plane-strain condition in MGs. They proposed that the existence of the elasto-plastic crack tip instability leads to a marked drop in the fracture toughness. These pioneer works provide an important foundation for a better understanding of the crack tip fields and the resultant fracture behavior.

The variability in the fracture toughness or plasticity of MGs is found to be the nature of processes occurring near the crack tip such as shear banding and crack branching, and thus results in different characteristic fracture morphologies (Lewandowski et al., 2005; Xi et al., 2005; Wang et al., 2006; Tandaiya et al., 2009; Xu et al., 2010; Ritchie, 2011; Wu et al., 2011; He et al., 2012; Narayan et al., 2014). From brittle MGs (e.g. Fe- and Mg-based) to ductile ones (e.g. Zr- and Pd-based), the fracture toughness can vary from ~1 s $MPam^{1/2}$ to ~100 s $MPam^{1/2}$ (Lewandowski et al., 2005; Demetriou et al., 2011; Xu and Ma, 2014). The crack initiation in brittle MGs is revealed to be stress controlled and involves cavity nucleation in front of the crack tip (Narayan et al., 2014). As is proposed that the cavitation stress and the hydrostatic stress ahead of crack tip determine whether brittle fracture via cavitation occurs or not in MGs (Singh et al., 2013, 2014). A misty-mirror morphology presents on the fracture surface of brittle MGs. Nanoscale patterns like dimple and periodic corrugation have been observed in the featureless mirror area (Xi et al., 2005, 2006), which indicates that even for MGs with ideal brittle behavior, the fracture still proceeds by a local softening mechanism but at different length scales. Xi et al. (2005) reported the dimple structures due to the highly localized strain and built a correlation between fracture toughness and plastic zone size. The quasi-brittle corrugation patterns are revealed to be the result of a random creation of cavities or voids in microscale (Xi et al., 2006; Wang et al., 2007). In contrast, the failure in ductile MGs is generally controlled by strain (Flores and Dauskardt, 2006), and the plastic zone accommodating plastic deformation around the crack tip exerts the most direct influence on it. The fracture surface in ductile MGs usually displays vein-like patterns. This typical pattern is ascribed to a Taylor instability process of a fluid meniscus (Spaepen, 1975; Argon and Salama, 1976). The stress softening caused by free volume creation and temperature rise is regarded as the physical reason for yielding and shear banding in MGs (Dai et al., 2005; Jiang and Dai, 2009; Dai, 2012; Greer et al., 2013), and it is naturally a major factor in the evolution of plastic zone. The experimental