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A 3D mechanistic model for brittle materials containing evolving flaw distributions under dynamic multiaxial loading

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ABSTRACT

We present a validated fully 3D mechanism-based micromechanical constitutive model for brittle solids under dynamic multiaxial loading conditions. Flaw statistics are explicitly incorporated through a defect density, and evolving flaw distributions in both orientation and size. Interactions among cracks are modeled by means of a crack-matrix-effective-medium approach. A tensorial damage parameter is defined based upon the crack length and orientation development under local effective stress fields. At low confining stresses, the wing-cracking mechanism dominates, leading to the degradation of the modulus and peak strength of the material, whereas at high enough confining stresses, the cracking mechanism is completely shut-down and dislocation mechanisms become dominant. The model handles general multiaxial stress states, accounts for evolving internal variables in the form of evolving flaw size and orientation distributions, includes evolving anisotropic damage and irreversible damage strains in a thermodynamically consistent fashion, incorporates rate-dependence through the micromechanics, and includes dynamic bulking based on independent experimental data. Simulation results are discussed and compared with experimental results on one specific structural ceramic, aluminum nitride. We demonstrate that this 3D constitutive model is capable of capturing the general constitutive response of structural ceramics.

1. Introduction

Defects control the mechanical response (and limit the applications) of brittle materials such as rocks, glasses, and ceramics. Pre-existing defects in brittle materials may be weak grain boundaries, triple junctions, second phases, inclusions, pores, and so forth. These internal flaws generally act as stress concentration sites that nucleate cracks, leading to catastrophic failure. This paper seeks to understand the dynamic failure of brittle solids through a physics-driven (mechanism-based) modeling approach.

The failure of brittle solids was first explored in geological research. Under macroscopic compressive stress fields, cracks were observed to initiate and start to grow, resulting in local open microcracks ("wing cracks") (Brace and Bombolakis, 1963; Schulson et al., 1991; Tapponnier and Brace, 1976). These open microcracks lead to volume change, generally termed dilatancy (Brace et al., 1966). Confining stress effects on rocks were also studied (Brace, 1964). Generally, a brittle–ductile transition was observed with increasing confinement (Gowd and Rummel, 1980), which was either attributed to fault

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formation (Byerlee, 1968), stable propagation of microcracks (Edmond and Paterson, 1972), or intracrystalline plasticity (Edmond and Paterson, 1972). These experimental observations provided early guidance to modeling work on brittle solids.

The *loading rate* has been shown to significantly affect the mechanical responses of brittle materials. Many ceramic materials (Chen and Ravichandran, 1996; Hu et al., 2012a, 2012b, 2011; Jiao et al., 2004; Kimberley and Ramesh, 2011a; Lankford, 1981; Paliwal and Ramesh, 2007; Staehler et al., 2000; Subhash and Ravichandran, 1998; Wang and Ramesh, 2004), geological materials (Frew et al., 2001; Green and Perkins, 1969; Kimberley and Ramesh, 2011b; Kumar, 1968; Li et al., 2005; Lindholm et al., 1974; Shan et al., 2000), and concretes (Bischoff and Perry, 1991; Grote et al., 2001) show an increase in strength when deformed at rates larger than a transitional strain rate.

In terms of *confining stress*, Heard and Cline (1980) conducted quasi-static confined experiments on BeO, Al_2O_3 and AlN and found that the peak strength increased with the confining pressure. They also observed an apparent brittle-to-ductile (BD) transition in BeO and AlN under highly confined compression. Chen and Ravichandran (1997, 1996) performed dynamic compression tests on AlN and a glass ceramic at strain rates up to 10^3 1/s, using a metal sleeve (the “shrink-fit” technique) to apply confining stresses during the dynamic loading. They also found a peak strength that increased with the confining stress, but did not observe a BD transition for AlN over their range of confinement. Paliwal et al. (2006) conducted dynamic planar confinement experiments on AlON and showed that dislocation plasticity was operative in the recovered AlON fragments. Hu et al. (2012a, 2011) conducted dynamic planar confined experiments on both hot-pressed and sintered AlN and found that (a) the failure process was shear-dominated under confinement, indicating a result of the microcrack interactions, and (b) dislocation activity was significant under confined dynamic loading conditions (Hu et al., 2012b).

Even higher (if non-uniform) strain rates are developed in shock experiments, together with high pressures, and so the rate-dependence and pressure-dependence of the strength of brittle solids can also be examined through characterization of the shock response. For example, aluminum nitride (AlN) has been characterized by Rosenberg et al. (1991), Kipp and Grady (1994a) and Dandekar et al. (1994). They noted that the shear strength was nearly independent of the shock stress for shock stresses above 8.1 GPa, suggesting plastic deformation mechanisms. This was later confirmed by TEM observations of dislocation activity within confined dynamic experiments (Hu et al., 2012b). Meanwhile, similar insensitivity of the shear strength to pressure was observed in alumina (Al_2O_3) by Bourne et al. (1998), Rosenberg et al. (1987), Grady (1998), Munson and Lawrence (1979) and Murray et al. (1998). Chen et al. (2006) observed twinning in alumina after shock stresses of 7.8 GPa, suggesting an additional inelastic deformation mechanism. Other structural ceramic systems, such as, aluminum oxynitride (AlON), boron carbide (B_4C), silicon carbide (SiC), and titanium diboride (TiB_2), have also been studied, and various inelastic deformation mechanisms have been hypothesized under shock loading conditions, i.e., amorphization (Chen et al., 2003), slip (Espinosa et al., 1992; Paliwal et al., 2008), twinning (Chen et al., 2006) and phase transformation (Kipp and Grady, 1994a). These inelastic deformation mechanisms should therefore be incorporated into constitutive formulations for these materials when addressing both high pressures and high strain rates.

Analytical models have also been developed to understand the mechanical response of brittle solids. Such models consider either pre-existing cracks affect the elastic constants of the brittle solid or how the cracks initiate and grow under general loading, leading to the failure of the brittle solid. In terms of the influence of cracks on elastic behavior, early work included that of Walsh (1965a, 1965b) and Budiansky and O'Connell (1976). Budiansky and O'Connell developed a relationship between the effective modulus and the damage, assuming open and randomly distributed cracks. Horii and Nemat-Nasser (1983) estimated the overall moduli of the cracked solid when crack closure and frictional sliding were involved. When the cracks were open, the model reduced to Budiansky and O'Connell's (1976) model. Nemat-Nasser and Obata (1988) built a 2D micromechanical model to capture the dilatancy and developed an anisotropic compliance tensor based upon the loading path without considering the interaction effects among cracks. Using the slip line theory (Schoenberg and Sayers, 1995) and a non-interaction approximation (NIA), Grechka and Kachanov (2006) obtained a relationship between the compliance increment and a tensorial damage parameter, providing a way to incorporate the damage anisotropy within the constitutive formulation.

In terms of the initiation and growth of cracks leading to failure, Costin (1983, 1985) developed a continuum damage model based upon the mechanics of microcrack nucleation and growth, including the interaction effects of collinear cracks. Ashby and Hallam (1986) and Horii and Nemat-Nasser (1986) independently developed seminal micromechanical models for compressive failure based upon a sliding crack to describe the splitting, faulting and brittle-to-ductile transition phenomena. They found that the crack development direction tended to align with the maximum principal loading direction, resulting in an “axial splitting” failure mode in compression, whereas when confining stress is applied, shear faulting occurs because of microcrack interactions and coalescence. Their micromechanical modeling work laid the foundation for most of the subsequent constitutive models for brittle solids. For example, the rate dependence of strength has been addressed through several derivative models (Huang and Subhash, 2003; Nemat-Nasser and Deng, 1994; Paliwal and Ramesh, 2008; Ravichandran and Subhash, 1995), most of which appeal to the inertia associated with dynamic crack growth. The density and size of the flaws influence the apparent transition strain rate as well as the strengths that can be achieved. The change in the macroscopic failure mode can also be described, for example, by a multiple-plane microcracking model which incorporates the damage induced anisotropy by pre-assigning discrete damage directions (Espinosa and Brar, 1995).

Other mechanisms have been incorporated in several ways. Rajendran (1994) and Rajendran and Grove (1996) utilized a set of microphysically based constitutive relationships to model deformation and damage processes in a ceramic, decomposing the strain into elastic, plastic and microcracking components. Deshpande and Evans (2008) developed a quasi-3D model for brittle solids by embellishing Ashby and Sammis (1990) micromechanics and adding lattice plasticity.