**Microscale Characterization of Fracture Nucleation and Associated Acoustic Emissions in Granite and Sandstone: Insights using the Discrete Element Method**

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**Abstract**

We develop dynamic micromechanical models of sandstone and granite to analyze fracture nucleation and propagation, causing seismic energy release during unstable failure. Calibrated models of rock are subjected to biaxial experiments leading to the development of a shear fracture through the progressive interaction of microcracks occurring in shear and tensile modes. Our models document a range of fracture growth patterns, providing insights into the source mechanisms of fracture energy released and volumetric changes in fracture gouge. Our models document that the growth of shear fractures in sandstone occurs through cooperative interaction between shear and tensile microcracks, with shear microcracks contributing heavily towards the release of fracture energy. While increase in confining pressure on sandstones does not result in increased microcracking activity, fraction of shear microcracking and associated energy increases, resulting in a transition from dilatant to compactant fracture zones in sandstones. The growth of shear fractures in granite occurs primarily through coalescence of tensile microcracks, with minimal shearing occurring in the fracture gouge. Increase in confining pressure on granite results in increased microcracking activity, dominantly in tensile mode. The increase in tensile microcracking with confining pressure results in larger acoustic energy release and formation of dilatant fracture zones in granite. The different mechanisms of fracture growth developed using micromechanical numerical models can help constrain the work budget during fracturing, geometry of fractures, source mechanisms of acoustic emissions, and failure forecasting techniques dependent on rock type.

1. **Introduction**

The mechanical loading of rocks results in local inelastic processes that produce microcracks [Kranz, 1983], and their cooperative interaction leads to formation of macroscopic fractures [Wong et al., 1997]. The growth of fractures results in the loss of cohesion and a reduction in rock strength, imparting permanent changes to the material. In addition, the introduction of fractures within a rock volume can modify porosity and permeability, affecting the transport properties of these materials. Finally, fracture energy is a major component of the work budget during rock deformation. The study of fracture energy is of relevance to industrial applications such as geothermal recovery, hydrocarbon extraction, safe design of nuclear repositories, as well as natural processes that accompany volcanism and earthquake generation. Thus, it is important to quantify the mechanisms of fracture growth and associated energy release.

The evolution of microcracks during rock deformation, and their evolution into macrofractures is a complex process influenced by lithology and associated rock strength [Menendez et al, 1996; Horii and Nemat-Nasser, 1985], porosity [Sulem and Ouffroukh, 2006] and confining pressure [Wong, 1997]. Microstructural analyses of rock fracture indicate that while fracture growth in crystalline rocks such as granite occurs largely through the coalescence of tensile microcracks [Brace et al., 1966; Moore and Lockner, 1995], resulting in the formation of dilatant shear bands [Walsh and Brace, 1984]. In weaker sedimentary rocks such as sandstone, pore collapse and shear microcracking have been shown to be the dominating mechanisms [Gallagher et al., 1974; Zhang et al, 1990], often resulting in the formation of compactant shear bands [Sulem and Ouffroukh, 2006]. The process of fracture growth is further influenced by the effect of confining pressure, which impedes dilatant deformation and favors non-dilatant processes. In granite, shear microcracking is observed to increase with confining pressure [Velde et al., 1993; Escartin et al., 1997], whereas a transition from dilating shear bands to compacting shear bands occurs in sandstone [Menendez et al, 1996; Besuelle, 2001]. While microstructural analyses help us build qualitative, observation-based models of fracture growth, they do not quantify the relative abundance of tensile and shear microcracks, and their influence on fracture energy, geometry and volumetric evolution of the shear fracture zone.

Recently, acoustic emissions have been employed to quantify the differences between proposed models of fracture growth. Acoustic Emissions (AEs) are broadly defined as high-frequency transient elastic waves generated by a sudden release of stored strain energy during fracturing of a rock [Lockner, 1993]. Unlike traditional integral rock damage indicators such as non-linear deformation and variation of elastic wave properties, the AE method offers the ability to detect individual fracture events, which contribute progressively to the deformation. The spatial and temporal microcrack distribution identified by AE’s has helped identify distinct stages of fracture initiation and coalescence, corresponding to the interplay between tensile and shear microcracks [Lei et al., 2006]. AEs also provide a quantitative measure of the work budget during rock deformation, and suggest that ~80-90% of input energy is released during growth of fracture in rock [Lockner et al, 1991; Goodfellow et al, 2015]. However, correlation between fracture energy and associated microcrack modes in laboratory studies may be complicated, for example, due to shear to compressional wave conversions [Modiriasari et al., 2017], difficulty in inverting AE’s for double-couple mechanisms [Jalali et al., 2018], and seismic attenuation [Ni and Iwamoto, 2002]. Distinguishing between tensile and shear microcracks is integral to balancing the fracture work budget, quantifying mechanisms of shear fracture growth, and determining how they affect volumetric changes in fracture zones.

The deformation during confined biaxial experiments and associated AE exhibit striking spatial and temporal similarity to earthquakes, obeying the Gutenberg-Richter relationship [Scholz, 1968] and Omori’s Law [Reasenberg and Jones, 1989]. The self-similarity in deformation from the laboratory to the field scale are particularly expressed in similar processes of rupture nucleation [Mitchell and Faulkner, 2008; Blenkinsop, 2008] and similar values of dimensionless, statistical seismic parameters [Hirata et al., 1987; Lei et al., 2004]. Since acoustic emissions accompanying brittle deformation show similarity over eight orders of magnitude of length [Hanks, 1992], understanding the variations in seismic amplitude and source locations from a micromechanical analysis can help characterize influence of lithology and confining pressure over catastrophic failure along faults.

Numerical methods provide the ability to monitor stresses and displacement of grains on a micro-scale, complementing the macromechanical behavior observed from microstructural and AE analyses. Discrete numerical methods are attractive to study brittle fracturing because, much like real rocks, the numerical materials are composed of assemblages of grains. Grain interactions yield emergent behaviors and heterogeneities form and evolve in response to changing stress conditions and material properties [Morgan 2015; LongJohn et al., 2018]. The grains are bonded to impart cohesion and simulate rock properties. Bond breakage, in response to applied boundary conditions, simulates microcracking allowing us to study the distribution and mode of individual microcracks and the bulk evolution of fracture and associated porosity. In this study, we use the Discrete Element Method [Cundall and Strack, 1979] to create and examine the behavior of sandstone and granite models in which cracks and fractures form spontaneously and release energy in the form of seismic waves. This choice of rock types will help us to compare the fracture growth mechanisms between weak, sedimentary rock (sandstone) and strong, crystalline rock (granite) of widespread interest. By monitoring microcracking activity, we seek to constrain fracture nucleation mechanisms, seismic energy release and volumetric changes in the fracture gouge during biaxial deformation experiments.

1. **The Discrete Element Method**

The discrete element method [Cundall and Strack, 1979] is a particle-based numerical technique that employs a time stepping, finite difference approach to solve Newton’s equations of motion for every particle in a system. The method first solves for forces imposed on the surfaces of each particle by neighboring particles or boundaries and then calculates a displacement based on the acceleration caused by sum of the forces. Particle motions are induced by external forces prescribed by stress or strain rate boundary conditions, and by forces resolved at interparticle contacts. The disequilibrium of forces drives particle displacements.

The Discrete Element Method (DEM) has been employed to simulate rock deformation from laboratory scale experiments to large scale geodynamic processes, including formation of deformation bands in sandstones [Wang et al.,2008], analyze changes in porosity and stress during biaxial experiments [Longjohn et al., 2018], evolution of fault gouges [Guo and Morgan, 2007], evolution of slope failure and landslide processes [Amitrano, 2006], and deformation of fold and thrust belts [Dean et al., 2013]. The numerical code used is RICEBAL, based on open-source code TRUBAL [Cundall and Strack, 1979]. RICEBAL resembles a numerical sandbox but offers added value by allowing material properties and mechanical states to be monitored throughout simulations and be correlated with deformation behavior and structure.

**2.1. Interparticle Contact Forces and Bonding**

Morgan, 2015 provides a detailed description of the mechanics of RICEBAL, which is summarized here. The force-displacement caused by particle interaction is characterized by normal and shear forces along elastic, frictional contacts, calculated using the following equations respectively [Fig. 1a]:

(Eq. 1)

(Eq. 2)

where *fn* is the repulsive normal force, *kn* is the normal interparticle stiffness, *δn* is the amount of overlap between particles in contact, *fs* is the shear force, *ks* is the shear stiffness, *δs* is the shear offset of particle centers. We implement the non-linear Hertz-Mindlin theory [Johnson, 1985] to calculate *kn* and *ks*, which are related to the elasticity of the particles the contact area of overlapping particles:

(Eq. 3)

(Eq. 4)

Where *Ep* is the Young’s Modulus of the particles, *Gp* is the Shear Modulus of the particles, and *Ra* and *Rb* are the radii of the respective discrete elements. In RICEBAL, *Gp* is an input parameter, which is related to *Ep* through the equation:

(Eq. 5)

Where *νp* is the Poisson’s ratio of particles. Shear forces at interparticle contacts are also limited by friction along particle surfaces (*µp*), as

(Eq. 6)

Where *fsmax* is the threshold force for particles to slide past each other. We implement interparticle bonding to impart cohesion into the material assemblage. The bonds have four key mechanical properties – *Eb*, the Young’s Modulus of the bond, *Gb*, the Shear Modulus of the bond, *Tb*, the tensile strength of the bonds, and *Cb*, the bond cohesion (unconfined shear strength of bonds at *fn*=0). The bonds connect the centers of particles in contact, and bond forces are at zero when particles are not displaced relative to each other (*δn*=*δs*=0). When particles are displaced in tension, the bonds support tensile and shear forces below predefined tensile strength and shear strength. When particles are displaced in compression, the bonds support the shear forces below the predefined shear strength. Normal and shear forces are related through the following equations [Fig.1b]:

In compression (*δn*>0): (Eq. 7)

In tension (*δn*<0): (Eq. 8)

Where *fnmin* is the minimum normal force required to break the bond. Bond-induced interparticle forces are calculated as

(Eq. 9)

(Eq. 10)

where *Ab* is the cross-sectional area of the elastic bond, assumed to be a circle with the radius equal to the smallest particle in contact. When particles are separated in tension (*δn*<0), bond tensile forces are limited by tensile strength and bond area, *Tb*\**Ab*. Shear forces separated during tension (*fn*<0) and compression (*fn*>0) are expressed by

(Eq. 11)

(Eq. 12)

**2.2. Particle Motions**

For each time step, net force, displacement, and moment are calculated by summing components of all contact forces acting on a particle. Net force (*Fp*) and net moment (*Mp*) are calculated for each particle by

(Eq. 13)

(Eq. 14)

Where *mp* and *Ip* are mass and moment inertia and *ẍp* and *Ӫp* are the linear and angular accelerations respectively. The particle displacements and roataions are calculated by inverting twice and integrating Eq. 14 and Eq. 15 over each time step for the new particle positions and orientations. At each time step, new particle configurations and contact forces are calculated. At each time step, particle motions are partially damped to dissipate energy in the system, to recreate the inelastic deformation in rocks [Cundall, 1987; Hazzard et al., 2000].

**2.3. Quantification of Stress, Strain and Porosity**

Sample volume, boundary stresses and particle positions through time are used to calculate bulk scale properties during biaxial experiments. The quantification of stress tensors during biaxial experiments using RICEBAL are explained in detail by Morgan, 2015. Membrane and platen boundary stresses correspond to the minimum and maximum principal stress (*σ3* and *σ1*). Membrane stresses are maintained constant at a specified confining pressure; the platen stresses are calculated by summing the net forces of the particles at each platen and dividing that sum by the platen area. Stress associated with bond breakage is recorded by dividing force at failure (fs or fn) by the area of the bond, which is equal to the area of the smallest particle in contact. The displacement of the platens is used to calculate axial strain (*εa*).

The quantification of bulk porosity during biaxial experiments using RICEBAL are explained in detail by Longjohn et al., 2018. Bulk porosity (*φ*) is calculated using total volume within the membranes and total volume of all the spheres within the sample as:

(Eq. 15)

1. **Methods**

In this study, we develop numerical analogs for Berea Sandstone and Lac du Bonnet Granite, representing two widely studied rock types ranging from weaker non-crystalline rocks to strong crystalline rock. We simulate biaxial experiments for both rock types to calibrate bulk behavior of numerical samples to experimental datasets under confined and unconfined conditions.

* 1. **Biaxial Experiments using the Discrete Element Method.**

We simulate samples as granular assemblage of ~60,000 particles with particle radii of 10-40 µm within an initial spatial domain of 0.04 m x 0.03 m. To prepare cohesive samples for biaxial experiments, we preconsolidate our samples to a confining pressure of 10 MPa. The two horizontal confining walls, constructed of rows of particles, are moved inward between rigid vertical walls of particles until preconsolidation stress of 10 MPa is achieved. After consolidation, sample dimensions are 0.019 m x 0.03 m. Porosity of all samples after preconsolidation is 0.176. Following preconsolidation, we reset the particles along horizontal platens to move independently in the vertical direction, while maintaining their constant confining stress, thus acting as a “membrane” that confines the sample during biaxial experiments. At this stage, we introduce interparticle bonds to simulate cohesive rock material. Axial compression is conducted by moving lateral platens inward at a constant velocity. As the vertical platens move inwards, local differential stresses increase, which causes failure of interparticle bonds, generating microcracks. With increasing deformation, the induced microcracks coalesce to form one or more shear fractures, ultimately resulting in the failure of the sample [Fig. 2a].

Biaxial experiments are run under confining pressures of 0, 2, 5,10,15,20,25,30,40 and 50 MPa. Macromechanical properties of the sample are collected at increments of 2000 cycles, associated with axial strain increments of 0.001 correspnding to incremental platen displacements of 0.008 mm. All simulations of biaxial experiments are conducted up to axial strain of 0.103.

* 1. **Calibration of Samples**

we simulate two rock types – Berea Sandstone and Lac du Bonnet Granite, which are defined by the propertiesthe within the assemblage.The micromechanical model properties are adjusted and the bulk behavior of our model materials is calibrated to replicate experimental laboratory data for Berea Sandstone and Lac du Bonnet granite. To capture the range of geomechanical rock behavior under both unconfined and confined conditions, we sought to reproduce to experimental datasets for Unconfined Compressive Strength (*UCS*), Young’s modulus (*E*), Mohr-Coulomb cohesion (*C*), and internal friction coefficient (*µ*),. The pertinent input microparameters include (1) mechanical properties of the particles - Shear modulus of particles (*Gp*), Poisson’s ratio of particles (*νp*), (2) mechanical properties of interparticle bonds - Young’s and shear moduli of bonds (*Eb* and *Gb*), tensile strength and cohesion of bonds (*Tb* and *Cb*), and (3) interparticle friction (*f*). The derived microparameters are determined indirectly by assigning values and comparing the response of the model to the geomechanical properties of the physical rock. The selected values of input microparameters that best reproduce the bulk properties of the two rock types are presented in Table 1. The calibration of numerical samples to experimental datasets is explained in detail in supplemental information, S1, and figures FS1 and FS2. The bulk behavior of numerical samples under confined and unconfined conditions is shown in Table 2, replicating the experimental geomechanical character of Berea Sandstone and Lac du Bonnet granite.

**3.3. Characterizing Microcracks and Acoustic Emissions**

To characterize the progression of fracture growth and associated material damage, we document several quantities and derive characteristic relationships that can be compared among experiments. Each bond breakage event is assumed to be a microcrack in the modeled rock samples. As axial stress is applied to the platens during the numerical biaxial experiments, fractures grow by the coalescence of emergent microcracks [Fig. 2b]. During each simulated biaxial experiment, we track the spatial and temporal evolution of microcracks and their mode of failure, and calculate the energy associated with each microcrack.

**3.3.1.** **Mode of Microcracks**

Interparticle bonds can fail in either tension or shear, as defined in Eq. 11-12. A tensile microcrack forms when interparticle normal stress exceeds the tensile strength of the bond, resulting in a mode 1 microcrack. Similarly, a shear microcrack results when local shear stress exceeds the shear strength of the bond in compression, resulting in a mode 2 microcrack. We document the mode of each microcrack generated, along with the failure stress at the time of bond breakage.

**3.3.2. Energy of Microcracks as Acoustic Emissions**

As axial stress is applied to the platens, interparticle bonds become distorted prior to failure, accumulating elastic strain energy. Bond failure that accompanies microcrack formation releases this energy instantly, emitting an acoustic signal analogous to an earthquake. The acoustic energy associated with each microcracking event is calculated using the following equation [Tang and Kaiser, 1998]:

(Eq. 18)  
Where *Ef* is the acoustic energy associated with a micro-fracture, *Cf* is the elastic modulus of the bond broken, *σcf* is the peak strength of the failed element and *vf* is the volume of microcrack. RICEBAL provides us with the ability to monitor stress associated with each broken bond *σcf*. Volume of a microcrack (*vf*) is taken as the sum of the areas of the two particles bounding the broken bond. If the microcrack fails in shear, *Cf* takes the value of shear modulus of the bond (*Gb*); if the microcrack fails in tension, *Cf* takes the value of Young’s modulus of the bond (*Eb*). Total fracture energy is calculated as the sum of energy from all microcracking events during a biaxial experiment, up to an axial strain of 0.103.

**3.4. Calculation of Damage Index**

Another measure of sample deformation is change in porosity. We measure the magnitude of porosity variations compared to the initial porosity using the Damage Index (*DI*). Since deformation during biaxial experiments becomes concentrated in the gouge zone of a shear fracture, the Damage Index helps characterize the volumetric changes induced by the fracture. For each biaxial simulation, we use the measured porosity (*φ*) at each increment of axial strain to calculate the Damage Index (*DI*) defined by Renaud et al., 2017 as:

(Eq. 19)

where *φi* is the porosity of the sample before the onset of the biaxial experiment. After preconsolidation to 10 MPa, the initial porosity of all samples in this study is 0.176. The Damage Index is an appropriate way to characterize the volumetric changes in the fracture zone since it eliminates the influence of initial porosity of rock. A positive value for *DI* at peak stress indicates the growth of a dilatant fracture zone, whereas a negative value of *DI* indicates a compactant and shear dominated fracture zone [Renaud et al., 2017].

1. **Results**

**4.1. Progressive Localization of Damage: Berea Sandstone**

As a first demonstration of our simulation results, we examine the growth of a macrofracture in Berea Sandstone under a confining pressure of 15 MPa. We identify four stages in the mechanical behavior as observed by the stress-strain behavior of the sample, and prescribed by experimental [Amitrano, 2003] and numerical studies [Longjohn et al., 2018]. Stage 1 (initiation), corresponding to an axial strain range from 0 to 0.023, is characterized by increasing rock strength and a linear stress-strain curve [Fig. 3]. This initial stage of the biaxial experiment is characterized by low microfracturing activity, 97% of which are generated in tensile mode. Microcracking activity during Stage 1 increases as axial strain on sample increases. Stage 2 (nucleation), corresponding to an axial strain range from 0.024 to 0.038, begins with the introduction of non-linearity in the stress-strain behavior of the sample until peak stress is reached. Stage 2 is characterized by increasing rock strength and decreasing slope of the stress-strain curve, corresponding to strain hardening behavior of the sample. Stage 2 of the biaxial experiment is characterized by very high microfracturing activity, generated in both shear (25%) and tensile (75%) modes. Microcrack growth increases as we approach peak stress of rock, marking the end of Stage 2. Stage 3 (rupture localization), corresponding to an axial strain range from 0.039 to 0.062, defines the post-peak stress-strain behavior of rock until residual strength of rock is attained. Stage 3 (localization) is characterized by decreasing rock strength corresponding to strain softening behavior of the sample. Stage 3 is characterized by high microfracturing activity, generated in both shear (19%) and tensile (81%) modes. Microcrack growth, especially in shear mode, declines as we approach the post-fracture residual strength of rock. Stage 4, corresponding to an axial strain range from 0.063 to 0.103, defines the frictional sliding behavior of the rock sample. Stage 4 (sliding) is characterized by nearly constant rock strength corresponding to the residual strength of rock. Stage 4 is characterized by very low microcracking activity, 94% of which are generated dominantly in tensile mode. Microcracking activity declines gradually as we approach the end of the experiment at an axial strain of 0.103. A total of 5442 microcracks developed in the sandstone sample deformed at a confining pressure of 15 MPa, with only 18% of them occurring in shear mode, generated mostly during Stage 2 and Stage 3 of the biaxial experiment.

The spatial distribution of microcracks generated during the four stages of the biaxial experiment show significant variation. Stage 1 is characterized by distributed tensile microcracking through the rock sample, indicating onset of dilatancy in the fracturing process [Fig. 2b]. Stage 2 is characterized by growth of shear and tensile microcracks, arising from the tensile asperities created in Stage 1. Shear microcracks generated in Stage 2 frequently occur as clusters, enveloped by tensile microcracks. During this nucleation stage, deformation is progressively localized as shear and tensile microcracks coalesce to form small fractures through the sample. Stage 3 is characterized by the coalescence of pre-existing microcracks and smaller fractures into a through-going shear rupture, assisted by newly generated shear and tensile microcracks. Microcracking activity during Stage 3 is very localized, with new asperities largely confined to the process zone of the developed shear fracture. Shear and tensile microcracks also coalesce to form smaller conjugate fractures, originating from the primary shear rupture. Stage 4 is characterized by shearing along the macrofracture surface. Microcracks are generated by the rupture of surface asperities and gouge fracturing, caused by plucking of grains along the shear fracture and associated conjugate fractures from sliding of fractured blocks of the rock. Thus, the nucleation and localization of fracture in sandstone is controlled by the cooperative interaction of tensile and shear microcracks. This indicates interplay between competing processes – dilatant tendencies from tensile microcracking and compactant tendencies from shear microcracking.

At *σ/σfailure*=1, we calculate a negative value of the Damage Index (*DI*), indicating a net decrease in volume of the sample [Fig. 4]. The abundance of shear microcracks in the fracture gouge, coupled with a calculated negative value of the Damage Index indicates the formation of a compactant fracture zone.

We calculate a total of 3.55 J of fracture energy released as AE during the biaxial experiment on Berea Sandstone under a confining pressure of 15 MPa to an axial strain of 0.103, exhibiting an exponential trend [Fig. 5]. AE energy release from microcracking activity during Stage 1 is small, contributing to 5% of the AE energy release. Stage 2 of the experiment, corresponding to the highest microcracking activity, is also associated with the highest release in fracture energy, with 49% of the total energy released as AE. Although, only 25% of the total microcracking from Stage 2 occur in shear mode, they contribute to 76% of the fracture energy released. Stage 3 of the biaxial experiment, corresponding to the coalescence of the shear fracture, is associated with release of 38% of the total fracture energy. While only 19% of all the total microcracking in Stage 3 occurs in shear mode but contribute to 75% of fracture energy released. Frictional sliding in Stage 4 results in a small amount of fracture energy release as AE. Stage 4 is associated with 7% a release of total fracture energy, with 39% released by microcracks occurring in shear mode.

Thus, the growth of shear fracture in Berea sandstone occurs through the cooperative coalescence of tensile and shear microcracks. While the abundance of shear microcracks is less than tensile ones, shear microcracking is localized in the fracture gouge and is the dominant mode of fracture energy release as AE. The nature of the fracture zone is controlled by the interplay between dilatant character of tensile microcracks and the compressive character of shear microcracks and imposed pressure.

**4.2. Progressive Localization of Damage: Lac du Bonnet Granite**

A comparison simulation to that described above is carried out on the numerical analog to the Lac du Bonnet Granite. The biaxial experiment, also conducted at 15 MPa confining pressure, results in some similar deformation trends as Berea Sandstone, but also some distinct differences, which are highlighted here. The growth of macrofractures in Lac du Bonnet Granite is dominated by tensile microcracking in four distinct stages [Fig. 6a]. Stage 1, corresponding to an axial strain from 0 to 0.007, is characterized by a linear stress-strain curve and rapid increase in rock strength attributed to the high Young’s Modulus of granite. Stage 2, corresponding to an axial strain range from 0.008 to 0.015, is the strain hardening phase of the experiment and is characterized by very high tensile microcracking activity as we attain peak strength of rock. Stage 3, corresponding to an axial strain range from 0.016 to 0.036, defines the post-peak strain-weakening behavior of rock, and is characterized by high tensile microcracking activity. Microcrack growth declines as we approach residual strength of rock. Stage 4, corresponding to an axial strain range from 0.037 to 0.103, defines the frictional sliding behavior of the granite sample and is characterized by residual strength of rock and low microcracking activity. A total of 2598 microcracks developed in the granite sample at a confining pressure of 15 MPa, with ~98% of them occurring in tensile mode generated largely during Stage 2 and Stage 3 of the biaxial experiment.

Stage 1 is characterized by distributed tensile microcracking through the rock sample, indicating onset of dilatant deformation in the sample [Fig. 6b1]. Stage 2 is characterized by growth of shear and tensile microcracks, predominantly around asperities created in Stage 1 [Fig. 6b2]. Shear microcracking during Stage 2 dominantly occurs in the process zone. As deformation begins to localize, small fractures are emergent. Stage 3 is characterized by the coalescence of pre-existing and newly generated microcracks and smaller fractures into a through-going shear rupture [Fig. 6b3]. Conjugate fractures, originating from the primary shear rupture are emergent at this stage, originating from coalescence of tensile microcracks in the gouge of the primary shear fracture. Stage 4 is characterized by shearing along the macrofracture surface [Fig. 6b4] and new microcracks are generated by gouge fracturing. Thus, the nucleation and localization of fractures in granite occurs through the coalescence of microcracks, predominantly generated in tensile mode. The abundance of tensile microcracking in the fracture zone indicates dilatancy as primary influence on the fracture gouge. As a result, we calculate very little compression due to confining pressure prior to failure, indicated by small negative values of the damage index [Fig. 4]. At *σ/σfailure*=1, we calculate a positive value of the Damage Index (*DI*), which along with the abundance of tensile microcracks in the fracture gouge indicate formation of a dilatant fracture zone.

We calculate a total of 21.91 J of fracture energy released as AE during the biaxial experiment on Lac du Bonnet granite under a confining pressure of 15 MPa, exhibiting an exponential trend [Fig. 6c]. The release of fracture energy in the four sequential stages of the biaxial experiment are 15%, 43%, 31% and 11% respectively. Through the entirety of the experiment, tensile microcracking is the dominant mode of energy release, contributing to 93% of the total AE energy. However, the small number of microcracks generated in shear mode (2% of total microcracks), correspond to events of high energy, contributing to 7% of total energy released. Thus, the growth of shear fracture in Lac du Bonnet granite occurs through the cooperative coalescence of microcracks predominantly generated in tensile mode. Fracture energy is largely released by microcracking in tensile mode. Since tensile microcracking is the primary mode of deformation, they compete with the imposed confining pressure to form dilatant fracture zones.

**4.3. Effect of Confining Pressure**

To examine how the behavior of each of these materials changes as a function of confining pressure, we carry out identical experiments on Berea Sandstone and Lac du Bonnet Granite models over a range of confining pressures. As we increase confining pressure from 0 MPa to 50 MPa on samples of Berea Sandstone, we observe an increase in peak strength of rock from 85.05 MPa to 238.82 MPa [Fig. 7a]. As confining pressure increases, rock strength increases, providing greater resistance to the formation of a shear fracture during biaxial deformation experiments. This increased resistance to fracture formation with confining pressure results in an increase in shear microcracks and a decline in tensile microcracks [Fig. 7b]. While the total number of microcracks created during biaxial deformation of sandstone does not vary significantly with confining pressure, microcracking in shear increases from 4% of total events at 0 MPa to 45% of total events at 50 MPa. The increase in shear microcracking and simultaneous decline in tensile microcracking indicates transition from dilatant fracture formation at low confining pressures to compactant fracture formation at high confining pressure. This observation is supported by the declining values of calculated Damage Index at *σ*/*σfailure* =1 with confining pressure [Fig. 7c]. At low confining pressures (0-10 MPa), we calculate positive values of the Damage Index at peak strength of rock, indicating formation of a dilatant fracture zone. At higher confining pressures (15-50 MPa), we calculate negative values of the Damage Index at peak strength of rock, indicating formation of a fracture zone dominated by compaction and shear. Total fracture energy released as AE increases from 1.73 J at confining pressure of 0 MPa to 7.97 J at confining pressure of 50 MPa, with the contribution of shear microcracking increasing from 31% to 92% [Fig. 7d]. The increase in fracture energy with confining pressure is due to increase in fraction of shear microcracking, which are associated with larger stress release during their formation.

Visual representation of microcrack locations in sandstone show an increase in microcrack distribution and fracture gouge thickness with confining pressure [Fig. 7e]. At low confining pressures, shear microcracks are concentrated in the fracture zone of the primary shear fracture and conjugate fractures. However, the distribution of shear microcracks increases with confining pressure as shearing becomes increasingly dominant mode of microcracking. In general, an increase in confining pressure also correlates with increase in number of conjugate fractures. The increase in confining pressure results in slower fracture coalescence and increase in events of shear microcracks, which are associated with high energy release. Thus, the increase in confining pressure on sandstone during deformation results in an increase in shear microcracking and associated AE energy, and the formation of compactant fracture zones,

As we increase confining pressure from 0 MPa to 50 MPa on samples of Lac du Bonnet granite, we observe an increase in peak strength of rock from 233.79 MPa to 433.63 MPa [Fig. 8a], indicating greater resistance to the formation of shear fracture during biaxial experiments. The formation of a fracture under increasing confining pressure is facilitated by an increase in total number of microcracks created during biaxial tests increases from 2110 at a confining pressure of 0 MPa to 3204 at a confining pressure of 50 MPa [Fig. 8b]. While number of shear microcracks increases slightly, the growth of the fracture is facilitated by a significant increase in tensile microcracking with confining pressure, indicating dilatant fracture zones in granite. Over a range of confining pressures from 0 to 50 MPa, we calculate positive values of Damage Index at *σ*/*σfailure* =1, indicating formation of dilatant fracture zones [Fig. 8c]. However, the dilatant tendencies of tensile microcracks are countered by the imposed confining pressure on rock resulting in a decline in rock volume with confining pressure. We calculate a decline in values of the Damage Index with confining pressure. Total fracture energy released as AE increases from 17.5 J at confining pressure of 0 MPa to 29.02 J at confining pressure of 50 MPa, with the contribution of shear microcracking increasing from 6% to 12% [Fig. 8d]. The increase in fracture energy with confining pressure is due to the rapid increase in number of tensile microcracks to form the shear fracture.

Visual representations of microcrack locations in granite show an increase in fracture gouge thickness with confining pressure [Fig. 8e]. The increase in resistance to fracturing from confining pressure is countered by increase in tensile microcracking activity in the gouge region of granite, resulting in nucleation of dilatant shear fractures. The increase in confining pressure on granite results in slower fracture growth due to coalescence of larger number of tensile microcracks. Thus, the increase in confining pressure on granite during deformation results in an increase in number of tensile microcracks and associated AE energy, and the formation of dilatant fracture zones,

1. **Discussions**

**5.1. Comparison of Fracture growth in Berea Sandstone and Lac du Bonnet Granite**

The formation of shear fractures in simulated sandstone and granite has similarities, but also some important differences that inform us about the mechanics of fracturing in these contrasting materials. Stage 1 (initiation), is characterized by distributed tensile microfracturing and low AE energy release in both rock types. During Stage 2 (nucleation), we observe very little shear microcracking in granite, whereas shear mode microcracking dominates in sandstone. Stage 2 is associated with the highest AE energy release for both rock types, however, the dominant contribution to release of fracture energy is tensile microcracking for granite as opposed to shear microcracking in sandstone. While shear microcracks generated in Stage 2 are localized to the zone of shear in granite, their distribution through the sample is much greater in sandstone, often extending beyond the fracture zone. Stage 3 (localization) is characterized by confined microcracking in the fracture zone in both granite and sandstone, but the two lithologies exhibit significant differences in mode of microcracks generated. While the growth of shear fracture is facilitated by the coalescence of tensile microcracks in, both shear and tensile microcracks are abundant in this phase of the experiment in sandstone. While release of fracture energy as AE remains high during stage 3, it is facilitated dominantly by tensile microcracks in granite as opposed to shear microcracks in sandstone. Stage 4 (frictional sliding) is characterized by tensile microcracking and gouge rupturing in both rock types, with low AE energy release. Since sandstone is mechanically weaker than granite, the stress required to generate asperities is lower. As a result, we calculate higher number of events and greater distribution of microcracks during biaxial deformation of sandstone in comparison with granite.

We infer different mechanisms of fracture nucleation in sandstone and granite. In weaker rocks such as sandstone, the growth of the fracture occurs through the progressive coalescence of shear and tensile microcracks [Fig. 9a]. The damage in the fracture zone is characterized by the interplay of dilatant and compactant tendencies of tensile and shear microcracks respectively. At low confining pressures, tensile microcracks dominate the fracture zone, resulting in the formation of a dilatant fracture zone. At high confining pressures, shear microcracking replaces tensile microcracking, resulting in the formation of a fracture zone dominated by compaction and shear. AE energy associated with fracture formation increases with confining pressure due to increase in shear microcracking. Shear microcracks are associated with a larger stress drop as they overcome both tensile and compressive forces during formation. Thus, the increase in shear microcracking with confining pressure results in an increase in AE energy in sandstone.

In strong rocks such as granite, the growth of fracture occurs predominantly through coalescence of tensile microcracks, resulting in formation of dilatant fracture zones [Fig. 9b]. As confining pressure increases, the increased resistance to fracture coalescence is countered by an increase in microcracking activity. AE energy increases with confining pressure on rock as number of tensile microcracks increases, resulting in an increase in fracture energy released as AE. The nature of fracture zone is an interplay between the dilatant tendency of tensile microcracking and compactant tendency of imposed confining pressure on rock.

**5.2. Validation of Models and Comparison with Experimental Datasets**

We test the validity of our model results by comparing our results to experimental datasets and highlight how our study can add to the current understanding of fracture formation. Our simulation results show that the growth of a macrofracture in Berea Sandstone occurs through the coalescence of microcracks occurring in shear and tensile modes, with the fraction of shear microcracks increasing with confining pressure [Fig. 7a]. The growth of shear fractures in sandstones has been shown to occur through coalescence of tensile and shear microcracks using AE source mechanism [Fortin et al., 2009] and microstructural analyses [Menendez et al., 1996]. Our simulation results show that the growth of shear microcracks occurs primarily in Stage 2 and 3 of a biaxial experiment, during the genesis and coalescence of the shear macrofracture as rock approaches its peak strength [Fig. 3]. The growth of microcracks in shear mode has also been shown to occur dominantly near the peak stress of the rock [Lei et al, 2004], with fraction of microcracking occurring in shear increasing with confining pressure [Baud et al., 2004]. However, there is little knowledge over how fracture energy is split between shear and tensile microcracks. Our simulation results add this body of work by showing that shear microcracks are the dominant mode of fracture energy release in weaker rocks such as sandstone, due to large stress drops associated with them during the nucleation and localization of shear fractures [Fig. 5]. The increase in confining pressure results in switch in mechanism, from dilatant to shear dominated [Fig. 7]. Thus, the increase in shear microcracking with confining pressure results in the greater AE energy observed in laboratory studies.

Experimental deformation experiments on Berea Sandstone show a transition from dilating to compacting fracture zones [Menendez et al., 1996; Besuelle, 2001]. Our simulation results show that the nature of the fracture zone is an interplay between the abundance of shear and tensile microcracks in the process zone. At low confining pressures, we observe dilatant fracture zones as tensile microcracks dominate the fracture and gouge region. At high confining pressures, the dominant damage mechanism is compactant, resulting in abundant shear microcracks in the fracture and gouge region. As a result, we observe compactant fracture zones in sandstones under high confining pressure conditions [Fig. 7c]. The switch in microcracking processes has been attributed to the decrease in internal friction with increasing confining pressure, as shear cracks are less pressure sensitive than tensile microcracks [Amitrano, 2003].

Our simulation results show that the growth and coalescence of a macrofracture in Lac du Bonnet granite occurs dominantly through the coalescence of tensile microcracks [Fig. 6a]. Similarly, the growth of fractures during biaxial experiments in granites has been shown to occur through coalescence of tensile microcracks using AE source mechanism [Lockner et al., 1991] and microstructural analyses [Peng and Johnson, 1972]. The increase in microcrack and AE energy with confining pressure has been experimentally observed granitic rocks [Stanchits et al., 2006]. Our model results show that the number of microcracks generated during biaxial experiments in granite increases with confining pressure in response to the increased resistance provided by confining pressure [Fig. 8b]. The increase in number of microcracks generated with confining pressure results explains the increase in AE energy release observed by experimental and numerical studies. Our results from deformation of granite samples also shows a small increase in shear microcracking with confining pressure, like behavior defined by granite in laboratory experiments [Jaeger et al., 2009]. Escartin et al., 1997 show a decline in dilatant nature of fractures in granite with increase in confining pressure. Our results reproduce this behavior [Fig. 8c], exhibiting a declining trend bulk dilation trend with confining pressure. The decline in dilatant nature of fractures is due to the pressure sensitivity of tensile microcracks, which close preferentially under high confining pressure, reducing the fracture porosity [Wong et al, 2001].

**5.3. Scale independence of Fracture Nucleation Mechanisms**

The deformation patterns during formation of shear fractures during biaxial experiments on samples are analogous to slip along faults [Lockner, 1993; Main and Meredith, 1989], particularly for shear faulting, which is supposed to be the main mechanism for earthquakes [Scholz, 1990]. Two widely acknowledged models of fracture propagation include the beam buckling model, proposed by Peng and Johnson, 1972, and the wing-crack model, proposed by Pollard and Segall, 1987. Peng and Johnson, 1972, through their beam buckling model suggest that faults evolve from an array of extensional microcracks. This mechanism is similar to the process of shear fracture growth recorded in our granite models. Pollard and Segall, 1987 suggest that both tensile and shear microcracks coalesce to form a fault of uneven surface. Field evidence and theory have shown that tensile fractures, referred to as wing-cracks, form around the tips of pre-existing asperities when loaded in shear, and the faulting occurs through the interaction of the extensional wing-cracks [Blenkinsop, 2008; Horii and Nemat-Nasser, 1985]. This deformation mechanism is similar to the process of shear fracture growth recorded in our sandstone models, which occurs through the progressive localization of shear and tensile microcracks. The differences occurring in deformation patterns of granite and sandstone models suggest that the process of fracture coalescence may be highly influenced by the mechanical properties of the lithology. AE associated with microcracking also shows remarkable statistical similarity to the seismic characteristics of earthquakes, obeying the Gutenberg-Richter relationship [Scholz, 1968] and Omori’s Law [Reasenberg and Jones, 1989]. In the following analysis, we will analyze the temporal variation in AE events and energy during biaxial experiments to understand and identify precursors to seismic growth and predict onset of fracturing using data driven techniques.

1. **Conclusions**

In this study, we employ the Discrete Element Method to capture key attributes of damage evolution associated with growth of shear fractures in sandstone and granite. We characterize the mode and acoustic energy associated with emergent microcracks during biaxial experiments to understand the various ways in which fractures evolve in different types of rocks. In sandstone, the growth of shear fractures occurs through the progressive coalescence of tensile and shear microcracks. While tensile microcracking is greater in number during the deformation of sandstone, the acoustic energy release is dominated by shear microcracking due to greater amount of stress release associated with each microcrack. At low confining pressures, tensile microcracks dominate the fracture gouge resulting in the formation of dilatant fracture zones. While the number of microcracks in sandstone does not show much variation as we increase confining pressure confining pressure, we transition from dilatant micromechanics to shear dominated micromechanics, resulting in the formation of compactant fracture zones. In granite, the growth of shear fractures occurs dominantly through the progressive localization of tensile microcracks, releasing fracture energy in the form of acoustic emissions. Since the fracture zone in granites is dominated by tensile microcracks, the fracture zone is dilatant in nature. As confining pressure on granite increases, the number of tensile microcracks increases and the nature of the fracture zone is an interplay between the dilatant nature of tensile microcracks and the compactant nature of confining pressure. Thus, we develop a micro-scale model of fracture growth in sandstone and granites by quantifying the spatial and temporal distribution of shear and tensile microcracks and quantifying their contribution to energy release.

**Figure Captions**

Figure 1: Mechanics of the Discrete Element Modeling implemented in this study.

Figure 2: Progressive evolution of spatial distribution of deformation due to microcracking in Berea Sandstone during biaxial compression test under confining pressure of 15 MPa. (a) Evolution of distortional strain in sample recording a sense of shear – the red color corresponds to negative values indicating right-lateral shear, and the blue color corresponds to positive values indicating left-lateral shear. (b) Spatial distribution of shear and tensile microcracks in sample, color coded to the axial strain at the time of formation.

Figure 3: Evolution of axial strain and microcracking events with axial strain in Berea sandstone during biaxial compression test under a confining pressure of 15 MPa: four distinct stages of deformation are identified. Deformation stages 1-4 correspond to axial strain of 0.0206, 0.0371, 0.0618 and 0.0969 complementing the spatial property distributions in Fig. 2. Fracture initiation (Stage 1) is due to growth of tensile microcracks, whereas fracture nucleation (Stage 2) and rupture (Stage 3) is facilitated by a combination of tensile and shear microcracks. Frictional sliding (Stage 4) is dominated by tensile microcracks along developed shear gouge.

Figure 4: Evolution of calculated Damage Index prior to onset of failure in Berea sandstone and Lac du Bonnet Granite during biaxial compression tests under confining pressure of 15 MPa. Deformation is characterized by compaction as differential stress is increased, followed by dilation when approaching failure. Berea Sandstone exhibits compactant character upon failure, whereas Lac du Bonnet granite exhibits dilatant character upon failure.

Figure 5: Evolution of AE energy from microcrack formation with axial strain in Berea sandstone during biaxial compression test under a confining pressure of 15 MPa. Shear microcracks correspond to 97% of total energy released during the experiment, dominantly released during nucleation and rupture (Stage 2 and Stage 3).

Figure 6: Evolution of microcracking, acoustic energy in Lac du Bonnet granite during biaxial compression test under confining pressure of 15 MPa. (a) Applied axial stress and AE events as a function of axial strain: four distinct stages of deformation are identified Deformation stages 1-4 correspond to axial strain of 0.0103, 0.0228, 0.0371 and 0.0927. (b) Spatial distribution of shear and tensile microcracks corresponding to Stages 1-4 highlighted in the biaxial experiment. (c) Evolution of AE energy from microcrack formation with axial strain. Tensile microcracks correspond to 93% of total energy released during the experiment, dominantly released during nucleation and rupture (Stage 2 and Stage 3).

Figure 7: Effect of Confining Pressure from 0 to 50 MPa on microcracking in Berea Sandstone during biaxial experiments to a final axial strain of 0.103. (a) Stress-Strain curves during biaxial tests show an increase in rock strength from 85 MPa to 235 MPa. (b) Total number of microcracks generated during biaxial tests does not show significant variation but the fraction of shear microcracks increases from 4% at 0 MPa to 45% at 50 MPa of confining pressure. (c) Evolution of Damage Index prior to failure indicates formation of dilatant fracture zones at low confining pressures (0-2 MPa) and compactant fracture zones at higher confining pressures (5-50 MPa). (d) Acoustic energy released during fracture formation increases from 1.7 J at 0 MPa to 7.8 J at 50 MPa with fraction of energy released in shear increasing from 31% to 92%. (e) Spatial distribution of tensile and shear microcracks shows increase in concentration of shear microcracks with confining pressure, indicating a transition from dilatant deformation processes to compactant deformation processes.

Figure 8: Effect of Confining Pressure from 0 to 50 MPa on microcracking in Berea Sandstone during biaxial experiments to a final axial strain of 0.103. (a) Stress-Strain curves during biaxial tests show an increase in rock strength from 234 MPa to 434 MPa. (b) Total number of microcracks generated during biaxial increases from 2110 at 0 MPa to 3204 at 50 MPa, facilitated by a rapid increase in number of tensile microcracks (c) Evolution of Damage Index prior to failure indicates formation of dilatant fracture zones at low confining pressures (0-2 MPa) and compactant fracture zones at higher confining pressures (5-50 MPa). (d) Acoustic energy released during fracture formation increases from 17.5 J at 0 MPa to 29.0 J at 50 MPa with fraction of energy released in shear increasing from 6% to 12%. (e) Spatial distribution of tensile and shear microcracks shows increase in number of tensile microcracks confining pressure, indicating dilatant deformation processes to overcome the effect of increasing confining pressure.

Figure 9: Variety of fracture nucleation mechanisms as axial stress is increased towards failure. Stages 1,2 and 3 correspond to the localized damage at the onset of yielding, localization and rupture respectively. (a) Growth of shear fracture in Berea sandstone through cooperative coalescence of shear and tensile microcracks, with fraction of shear microcracks increasing with confining pressure. Dilatant fracture zones are calculated for low confining pressures (0-2 MPa) and compactant fracture zones are calculated for higher confining pressures (5-50 MPa) [Fig. 7c]. (b) Growth of tensile shear fracture in Lac du Bonnet granite through cooperative coalescence of primarily tensile microcracks. Dilatant fracture zones are calculated for confining pressures from 0-50 MPa due to abundance of tensile microcracking [Fig. 8c].

Supplementary Figure 1: Unconfined macromechanical properties of calibrated DEM materials used in this study. Berea Sandstone model has a Young’s Modulus of 4.28 GPa and unconfined compressive strength of 85 MPa. Lac du Bonnet granite model has a Young’s Modulus of 42.47 GPa and unconfined compressive strength of 234 MPa.

Supplementary Figure 2: Mohr-Coulomb properties of calibrated DEM materials used in this study. Berea Sandstone model has a cohesion of 29.3 MPa and an angle of internal friction of 29 degrees. Lac du Bonnet model has a cohesion of 54.6 MPa and an angle of internal friction of 40 degrees.