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Key Points:

- A numerical model is established with a priori vein geometry to correspond to a prototype of granite that contains authigenic veins
- Influences of in situ stresses, vein strength, and vein geometry on rupture characteristics of veined granite are examined
- Soft veins localize rupture in contrast to hard veins, which impede localized rupture resulting in the formation of conjugate shear bands

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Rupture Of Veined Granite In Polyaxial Compression: Insights From Three-Dimensional Discrete Element Method Modeling

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Abstract Granite formations have been frequently involved in subsurface energy-related activities such as radioactive waste disposal, oil, and gas storage. This is principally because of their mechanical stability, low permeability, and high corrosion resistance. These favorable properties, however, can be compromised by the addition of mineral veins, which tend to occur ubiquitously in upper crustal rock formations. Evaluation of the impact of veins on the integrity and rupture characteristics of granite, especially under true triaxial stresses, is therefore important yet currently underemphasized. This study examines the rupture of veined granite in polyaxial compression via a discrete element method model. In the model with soft veins, the rupture is localized along the fabricated inclined veins (45° relative to the horizontal with strike running in the σ_2 direction) under low confining stresses ($\sigma_2 < 67$ MPa); in contrast, a combined rupture of veins and granite matrix is observed when σ_2 is increased to 141.6 MPa. Shear sliding along the inclined veins is revealed by examining the displacement field. Shear-induced volumetric dilation is suspected in the soft-veined models in relatively low confining stresses ($\sigma_2 < 67$ MPa) with sliding and dilation behavior apparently suppressed at $\sigma_2 = 141.6$ MPa. Hard veins impede local rupture, resulting in conjugate shear bands. The well-recognized σ_2 effect is observed for the hard-veined models, while no pronounced σ_2 effect is noticed for the soft-veined models. This study also reveals that vein thickness has a negligible impact on rupture characteristics, which is however profoundly affected by vein orientation.

1. Introduction

Granite is one of the most common rocks in the Earth's crust. Because of its favorable mechanical, hydrogeological, and geochemical properties, granite formations have been frequently involved in the subsurface energy-related activities such as long-term disposal of radioactive waste (Mariner et al., 2011) and underground storage of oil and gas (Lee et al., 1996; Lindblom, 1978; Wang et al., 2015). Granite, by its nature, is heterogeneous since it is made up of various mineral aggregates (basically quartz, feldspar, and mica) with distinctive texture and chemical compositions. The addition of mineral veins that tend to be ubiquitous in the upper crustal rocks further enhances the heterogeneous nature of granite. The veins are geological features that form when the minerals within fluids in fractured rocks are deposited. Because of their distinctive mechanical properties compared with that of granite, veins can modulate the overall geomechanical behavior and integrity of rock (Gale et al., 2007). Understanding how the veins affect the mechanical characteristics of granite in in situ stress conditions is of potential importance for evaluating the integrity and permeability evolution of veined granite, thereby maintaining a safer, purposeful, and environmental-friendly underground energy storage environment.

Unlike mechanical discontinuities, mineral veins may exhibit considerable tensile strength (Shang et al., 2015). Veins that are weaker than the host rock can be fractured under external stresses (Virgo et al., 2013; Lee et al., 2015; Shang et al., 2016). Figure 1a shows an example of a weak calcite vein (~150 mm thick) sandwiched by the Horton siltstone formation (England). The calcite veins exhibited various geometries probably due to tectonic activities (Figure 1b), with evidence of fracturing along a soft vein within a siltstone block shown in Figure 1c.

Figure 1. (a) An ~150-mm-thick calcite vein sandwiched by the Horton Formation (siltstone), England, (b) distortion of the calcite veins due to tectonic activities, and (c) fracturing along a soft vein within a siltstone block. (d) A Bukit Timah granite core (Singapore) contains hard quartz veins with different orientations, and (e) a small stick of core was detached from the whole core due to mechanical load. The vein traces observed on the surface of the Bukit Timah granite core (d) was used as a prototype in the establishment of the numerical model.

Experimental studies that explore the effect of veins on the rupture (The term “rupture” used in the study follows the definition in Bieniawski (1967), which refers to a type of failure where a structure (e.g., a rock specimen) disintegrates into two or more pieces.) characteristics of rocks are rare. This is probably due to the intrinsic complexity of natural veins and tectonic activities (McBeck et al., 2019), making it difficult to prepare natural-veined samples in the laboratory. This implies that the experimental results based on a particular veined sample are often nonreproducible. Although rare, a few papers illustrate this point. For example, Lee et al. (2015) reported a laboratory semicircular bend study of the influence of weak calcite veins on opening-mode fracture propagations. Shang (2016) presents a comprehensive laboratory study of the direct

tensile properties of cylindrical siltstone samples containing single veins. Although difficult, the effect of multiple veins on the mechanical behavior of rock is also explored. An attempt in the construction of discrete vein networks considering vein geometry (i.e., vein thickness and orientation) was reported by Turichshev and Hadjigeorgiou (2017), where up to thirty-three visible vein exposures were traced on sixteen 50-mm diameter cores in the laboratory. The traced veins were then implemented into a 3D representation of vein networks by assuming that the vein traces were persistent within the cores. The thickness of each vein was measured at a minimum of two locations; the measured vein thickness was varied between 0.2 and 16.6 mm, which follows a power law distribution. The vein orientation with respect to the loading axis was recorded for each vein. The results of a statistical analysis show that the veins were oriented at multiple orientations, from subparallel to subnormal, without preferred distributions.

Although many veins can be involved within a rock block or a specimen, the rupture of veined rock is often controlled by critically oriented veins, as demonstrated by Turichshev and Hadjigeorgiou (2015), who experimentally probed the rupture characteristics of veined andesite specimens using conventional triaxial experiment. The results of their study demonstrated that the rupture of veined rock often occurred along an individual vein or a combination of veins that were oriented at angles of approximately 50°–70° with respect to lateral stress orientation. The conclusion, however, is only applicable to cases where the strength (e.g., uniaxial tensile strength) of the adversely oriented veins was lower than that of the host rock. It appears virtually impossible from a practical standpoint to conduct a sensitivity study in the laboratory to understand the impact of vein parameters (e.g., thickness, orientation, and strength) on the mechanical behavior of rock due to the irreproducibility of the extreme conditions of temperature and pressure required for natural vein formation.

To overcome the experimental limitations, numerical methods have been used to systematically understand the influence of veins on the failure and microstructural characteristics of rocks. For example, Virgo et al. (2013) established a discrete element method (DEM) model to study the influences of both vein orientation and strength contrast between the vein and host rock on the fracture behavior of veined rocks. Their model contained a single vein with a priori tabular geometry and a predefined notch to allow fracturing, and their simulation was performed under uniaxial unconfined extension. They concluded that for veins that are weaker than the host rock, fracturing is localized within the vein material, whereas for stronger veins, failure of veined rock tends to initiate along the vein-rock interface or within the rock matrix, depending both on the strength contrast of vein, host rock, and vein-rock interface and on the orientation of the vein relative to the stress field (Virgo et al., 2013). Following on from the study (Virgo et al., 2013), a workflow that consists of deformation simulation (model fracturing), stress relaxation, and sealing and rotation was produced to mimic repeated fracturing and crack sealing under more realistic boundary conditions (Virgo et al., 2014). A comparison study of the effect of the two previously used boundary conditions on the failure mechanisms was then reported in Virgo et al. (2016). Ankit et al. (2015) produced a phase field model of bitaxial sealing in quartz veins and concluded that both vein geometry (e.g., aperture and shape) and properties of vein-filling materials (e.g., mineralogy and grain size) can affect the evolving microstructure.

Despite the above contributions, their investigations are limited to relatively simple stress conditions. In reality, rock behaves differently under polyaxial confinement, the magnitude and orientation of which can be affected by many factors such as tectonic activities (Huang et al., 2016; Scholz, 2015), hydrological loading (Lu et al., 2018), and anthropogenic activities (Segall & Lu, 2015; Siren et al., 2015). The stress state in the three-dimensional space is generally represented by three mutually perpendicular principal stress components (i.e., σ_1 , σ_2 , and σ_3), where σ_1 represents the maximum principal stress, σ_2 the intermediate principal stress, and σ_3 the least principal stress (the stress is positive in compression and negative in tension). The stress condition $\sigma_1 > \sigma_2 = \sigma_3$ defines the conventional triaxial stress state (often termed triaxial compression [TC]); the stress condition $\sigma_1 > \sigma_2 > \sigma_3$ represents the true triaxial stress state (i.e., polyaxial compression [PC]).

Extensive experimental, analytical, and numerical studies have demonstrated that σ_2 has a significant influence on the rock failure characteristics (Crawford et al., 1995; da Fontoura, 2012; Duan et al., 2017; Feng et al., 2019; Haimson, 2006; Ma & Haimson, 2016; Mogi, 1967; Mogi, 1971; Priest, 2012; Schöpfer et al., 2013; Wiebols & Cook, 1968; Zhang & Zhu, 2007). For a given constant σ_3 , σ_1 at the failure of a rock (i.e.,

$\sigma_{1, \text{peak}}$) often increases with the increment of σ_2 to a maximum magnitude and then decreases to a value just greater than its conventional compressive strength (Cai, 2008; Feng et al., 2019; Pan et al., 2012). This evolutionary trend was often termed as the σ_2 effect. The fracture plane within the rock is often oriented in the direction parallel to σ_1 - σ_2 , due to the relatively high confinement of σ_2 compared with that of σ_3 (see Haimson, 2006 for a review on this topic).

Although the importance of σ_2 has been known for more than 50 years, previous polyaxial experiments mainly dealt with intact rocks (Artkhonghan et al., 2018; Crawford et al., 1995; Feng et al., 2019; Mogi, 1967; Haimson, 2006; Hecker & Petrovic, 1981; Ma & Haimson, 2016). So far, no previous publications, at least to the best of the author's knowledge, have ever addressed the questions associated with the geomechanical response of veined rock in PC. It is still unclear whether the well-recognized rupture patterns observed based on intact rocks is applicable to ubiquitous veined rocks.

To address the aforementioned challenges, in this study, a three-dimensional DEM model of veined granite was developed, with the overall objective of exploring the rupture characteristics of the veined granite in PC. The DEM model enables the synthetic reproduction of natural-veined rocks with identical vein properties that parallel the mechanical behavior in polyaxial tests. The model also allows a detailed examination of the effects of vein strength, geometry, and in situ stress conditions. By using the three-dimensional DEM approach, this work addresses (1) rupture of veined granite and the evolution of microcracks in PC; (2) effects of the mechanical and geometrical properties of veins on micromechanics, rupture pattern, and overall strength of veined granite; and (3) comparison of the numerical results and corresponding predictions from classic failure criteria. It is expected that the results of this work show clues for the significance of mineral veins on the control of granite integrity in true triaxial stresses and can potentially improve our understanding of the evolution of stability problems associated with the subsurface energy-related applications.

2. Material and Methodology

2.1. Veined Bukit Timah granite

The Bukit Timah Granite, formed from a large body of intruded acidic magma in the early to middle Triassic (250–235 Myr) (Wu et al., 2000), covers around one third of Singapore island. It is recognized as the base rock of Singapore since it overlies other formations such as Jurong Formation and Old Alluvium. Bukit Timah (BT) granite, predominantly found in the Bukit Timah Granite formation, is commonly thought to be a source rock with energy storage and geothermal energy potential in Singapore (Williams & Eubank, 1995; Hamza et al., 2008; Oliver, 2009). The granite is normally light gray (sometimes pinkish) and medium-to-coarse grained, with an average uniaxial compressive strength (UCS) of ~186 MPa (Zhao, 1996). It is composed mostly of quartz (30%), feldspar (60%–65%), biotite, and hornblende (<10%) (Cai, 2012; Wu et al., 2000).

A special feature that is often observed in BT granite is crack-sealed mineral veins, which is suspected to have a significant impact on the integrity and geomechanical behavior of the rock. Figure 1d shows a piece of cylindrical-veined BT granite core that was collected from a borehole (up to 200 mm below the surface of the Earth) drilled at the Gali Batu area in Singapore. The veined granite core contains authigenic cement (veins): two subvertical veins, one inclined vein and one subhorizontal vein. A small block was disassembled from the core along a relatively weak vein (Figure 1e). The vein geometry observed on the surface of the granite core was used as a natural prototype in the establishment of the numerical model.

2.2. Particulate DEM

The particulate DEM approach is becoming increasingly popular in both research and practice in the many fields such as geomechanics, rock mechanics, and petroleum engineering. In this work, the bonded particle model in the particle flow code (PFC 3D) was used to simulate the BT granite and the vein-filling minerals. The main advantage of particulate DEM over continuum-based methods (e.g., finite element method) is that DEM can capture fracture initiation, propagation, and coalescence in exquisite detail at both microscale and macroscale, without the need of constitutive laws (PFC3D manual, 2008; Potyondy & Cundall, 2004).

The basic principle of DEM is to mimic a geomaterial such as rock as an assembly of rigid particles, and the Newton's second law provides the fundamental relation between particle motion and the forces generated between the particles (Cundall & Strack, 1979; Potyondy & Cundall, 2004). The particles in the DEM approach are assumed to be a disk (2D) or a sphere (3D) to simplify the process of particle contact

detection and the calculation of normal and shear forces between the particles. These particles can overlap at their contact points, this feature being used to model the contacts occurring between two real physical objects (O'Sullivan, 2008). For the parallel-bonded particle model (in PFC 3D), a force and a moment are developed within bond materials, and the force and moment can be related to maximum normal and shear stresses acting on contacting particles (PFC 3D manual, 2008). The cohesive bond will break and vanish once either of the maximum stresses exceeds its corresponding bond strength, and the fracture propagation can be achieved by the coalescence of multiple bond breakages (Lisjak & Grasselli, 2014; Shang, Duan, et al., 2018). The shear force between particles after the bond breakage arises from the coefficient of friction at their contacts, and its magnitude also depends on the normal force between the particles. In this study, the localized failure of a bond (at a point) at microscale is expected to occur firstly in the particle-based DEM model, prior to the formation of macroscopic rupture planes (i.e., coalescence of the microscopic failed bonds), leading to the loss of strength of the entire model.

2.3. Polyaxial Test Setup

In this work, cubic DEM models were densely packed within vessels with a constant dimension of $60 \times 60 \times 120$ mm (see Figure 2a, around 133,871 particles were generated). To generate an identical model, these particles with a uniform particle size distribution (0.6–0.996 mm in radius) were randomly generated under a constant random value (10,005). The identical packing of the particles allows the sensitivity of parameters (e.g., stress paths, vein thickness, vein orientation, etc.) to be investigated. To obtain an approximate quasi-static condition for the granite model, a damping coefficient of 0.7 was used to dissipate kinetic energy in each computational cycle (Potyondy & Cundall, 2004).

Two vertical veins, one horizontal vein and one inclined vein, were generated inside the DEM model (Figure 2a, light bands), and the vein orientation and their relative position generally follows a real observation of the vein traces exposed on a veined granite core (Figure 1d). For the inclined vein, the vein thickness (t) and the vein orientation (β) remained constant in the early part of this work, which were 5 mm and 45° , respectively. To understand the effect of vein thickness and orientation on the rupture characteristics, in the latter part of this work more simulations were conducted by varying the vein thickness and orientation of the inclined vein. Four thickness values ($t = 8, 12, 16$, and 20 mm) and four orientation angles ($\beta = 15^\circ, 30^\circ, 60^\circ$, and 75°) were considered in the study.

Three stress conditions were documented in the literature, which include TC ($\sigma_1 > \sigma_2 = \sigma_3$), PC ($\sigma_1 > \sigma_2 > \sigma_3$), and triaxial extension (TT; $\sigma_1 = \sigma_2 > \sigma_3$). The Lode parameter (μ) was used to quantitatively correlate the three principal stresses and describe the three stress conditions (Artkhonghan et al., 2018; Riley et al., 2006),

$$\mu = (2\sigma_2 - \sigma_3 - \sigma_1) / (\sigma_3 - \sigma_1), \quad (1)$$

where $\mu = 1$ for TC, $-1 < \mu < 1$ for PC, and $\mu = -1$ for TT.

In the study, the TC and TT were only applied on intact granite models for verification of the DEM model. All the veined granite models were deformed in PC to mimic the real stress conditions in the subsurface. Boundary conditions were controlled via three independent stresses and applied by using frictionless walls (for clarity, the walls are not shown in Figure 2a.). The loading path mainly comprises three stages: (1) Hydrostatic confinement is applied on the model ($\sigma_1 = \sigma_2 = \sigma_3$) until the predefined σ_3 is achieved (Figure 2b); (2) damping of the model is then conducted to dissipate kinetic energy for achieving a quasi-static condition prior to PC; (3) the cubic DEM models are then deformed with a constant velocity (-0.02 m/s in the negative z -axis direction and 0.02 m/s in the positive z -axis direction) in the σ_1 direction until model rupture (Figure 2a). In the meantime, the σ_3 is remained constant, and the σ_2 is varied against σ_1 to maintain a constant Lode parameter μ (equation (1)). This novel stress path (Figure 2b), with the help of Lode parameter (equation 1), allows complete stress conditions (i.e., TC, PC, and TT) to be considered. In this study, σ_1 is increased until it reaches a peak ($\sigma_{1, \text{peak}}$), indicating sample rupture. The simulation is terminated once σ_1 decreases to $80\% \sigma_{1, \text{peak}}$, so that a complete stress-strain curve can be logged in the simulation.

2.4. Strength Contrast of Veins and Granite and Model Calibration

The strength contrast of vein-filling minerals and their host rocks is often recognized as the most important parameter that controls the fracture characteristics (Cook et al., 1964; Virgo et al., 2013, 2014). In this work,

Figure 2. (a) Numerical setup for the polyaxial compression test on a veined Bukit Timah granite model with a dimension of $60 \times 60 \times 120$ mm ($\sim 133,871$ particles; green particles represent rock matrix, and light bands mimic veins). The thickness of the inclined vein (t) remained constant (5 mm) in cases 1–3 and was varied (8, 12, 16 and 20 mm) in case 4 (Table 1). The orientation of the inclined vein (β) remained constant (45°) in cases 1–3 and changed (15° , 30° , 60° , and 75°) in case 4 (Table 1). (b) A novel loading path was applied on the model, where σ_3 was constant in each simulation, σ_2 was increased with the increase in σ_1 to maintain a constant Lode parameter. Four different σ_3 levels (0, 3, 10, and 30 MPa) were involved in the simulation.

both hard and soft minerals compared to that of BT granite were considered. The vein-filling minerals were assumed to be homogeneous. To produce veins that have different strengths and a clear physical meaning, quartz stands for the hard mineral, and calcite represents the soft mineral. The selection of the two representative minerals yields a distinct strength contrast of the vein and the host rock in the established DEM model.

The mechanical properties (UCS = 186 MPa, Young's modulus = 73.9 GPa, Poisson's ratio = 0.16) of the BT granite reported in Zhao (1996) were used in the host rock strength calibration. To mimic quartz and calcite, their UCS values were deduced from hardness, and the deduced UCS values were used in the microparameter calibration. Because the UCS values of rock-forming minerals are not available in the literature, instead, the hardness of mineral is frequently reported (Pellant, 2002). In addition, several experimental studies have demonstrated that hardness is linearly correlated with the UCS of brittle or crystalline materials (Aliyu et al., 2019; Grigg, 2016; Hucka & Das, 1974; ISRM, 1981; Kahraman et al., 2012; Zhang et al., 2011). The hardness was therefore used to estimate the UCS of the homogeneous vein-filling minerals (i.e., quartz and calcite), thus allowing the calibration of microparameters of the veins. The Vickers hardness of granite, quartz, and calcite are about 850, 1,161, and 157 kg/mm², respectively (Hasirci & Hasirci, 2018; Lewis et al., 2003).

In the calibration process, a trial-and-error process was used, and the procedure was similar to that used by Shang, Zhao, et al. (2018). In the calibration of the microparameters of granite, the modulus of the particles and bond was first calibrated, followed by the calibration of normal to shear stiffness ratio. Finally, the bond cohesion, bond tensile strength, and bond friction angle were fine tuned to match the UCS of the BT granite. The calibration of the microparameters of quartz and calcite minerals also involve a trial-and-error process to ensure the strength contrast of the veins and to ensure that host rock can match their respective hardness ratios (quartz/granite = 1.37 and calcite/granite = 0.18). The calibrated parameters are freely available (see Acknowledgements).

It should be noted that in this study, the parallel bond contact model in the PFC 3D was assigned to all particles forming the veins, rock matrix, and vein-rock interfaces, to make sure that the strength values of their microparameters are comparable. For simplicity, the vein-granite interface parameters were set to be the same as that of granite for the soft-veined models and as that of quartz for the hard-veined models. The

assumption used in Lee et al. (2015) was also employed, which states that the granite, calcite, and quartz vein minerals share the same Poisson's ratio (0.16). The strength contrast of the veins and the host rock was reflected by the difference of their bond tensile strength and bond cohesion. It is acknowledged that not considering the contrast in the Poisson's ratio of veins and granite may lead to a non-negligible discrepancy; variations in Poisson's ratio will be investigated in the next phase of this project.

2.5. Numerical Scenarios and Post Processing

Four different numerical scenarios were investigated in this work (see Table 1).

2.5.1. Intact BT Granite Without Veins (Case 1)

In case 1, numerical tests in all three stress conditions including TC ($\mu = 1$), PC ($\mu = 0.5, 0$, and -0.5), and TT ($\mu = -1$) were carried out on the intact BT granite models (Table 1). For each stress condition, four constant σ_2 levels (0, 3, 10, and 30 MPa) were applied; thus, a total of twenty numerical simulations were conducted in this scenario. The main aim of designing this scenario is to evaluate the robustness of the DEM model through assessing the rupture characteristics of intact rocks in various stress conditions and comparing the numerical results with corresponding predictions from two well-recognized failure criteria, that is, the Mogi criterion (Mogi, 1971) and modified Lade criterion (Ewy, 1999; Lade, 1977).

The three-dimensional Mogi criterion (Mogi, 1971) was used to estimate $\sigma_{1, \text{peak}}$ under different combinations of σ_2 and σ_3 . The Mogi criterion defines the octahedral shear stress (τ_{oct}) in terms of the effective mean stress ($\sigma_{m,2}$) using a power relation:

$$\tau_{\text{oct}} = k\sigma_{m,2}^n, \quad \tau_{\text{oct}} = \frac{1}{3} \sqrt{(\sigma_{1, \text{peak}} - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_{1, \text{peak}})^2}, \quad (2)$$

$$\sigma_{m,2} = (\sigma_{1, \text{peak}} + \sigma_3)/2, \quad (3)$$

where k and n are Mogi material constants, which are empirical and can be determined from polyaxial experiments. It is often found that $k > 1.5$ and $n < 1$, based on existing true triaxial test, results on various rock types (dolomite, limestone, trachyte, sandstone, siltstone, amphibolite, marble, shale, and granite) (Al-Ajmi & Zimmerman, 2005).

The Lade criterion was originally proposed for soils that have zero or very low cohesion (Lade, 1977) and then modified to consider cohesive materials such as concrete and rocks (Kim & Lade, 1984). Ewy (1999) presented a simplified version of the Lade criterion that can be expressed by equation (4).

$$\left(\frac{I_1^3}{I_3} \right) = 27 + \eta, \quad (4)$$

$$I_1 = (\sigma_{1, \text{peak}} + S_a - P_p) + (\sigma_2 + S_a - P_p) + (\sigma_3 + S_a - P_p), \quad (5a)$$

$$I_3 = (\sigma_{1, \text{peak}} + S_a - P_p)(\sigma_2 + S_a - P_p)(\sigma_3 + S_a - P_p), \quad (5b)$$

where S_a and η are material parameters, which should be determined to describe the rock strength; these two parameters can be calculated from equations (6) and (7). P_p is the pore fluid pressure, which is zero in this study because the pores in our model are not filled with fluids.

$$S_a = \frac{c}{\tan \varphi}, \quad (6)$$

$$\eta = 4(\tan \varphi)^2 \left(\frac{9 - 7 \sin \varphi}{1 - \sin \varphi} \right), \quad (7)$$

where c is the cohesion and φ is the friction angle in the Mohr-Coulomb failure criterion.

The modified Lade criterion is attractive to employ because the material constants in this criterion can be directly related to cohesion and friction angle (Equations (6) and (7)) of a targeted material. There is therefore no need to perform TC experiments to determine the material constants.

Table 1
Description of the Four Numerical Scenarios Examined in This Work

Numerical scenarios	Sample	Number of simulations	Lode parameter, μ	Minimum principal stress ^a	Purpose
Case 1	Intact granite	20	$\mu = 1$ (TC) $\mu = 0.5, 0, -0.5$ (PC) $\mu = -1$ (TT)	$\sigma_3 = 0, 3, 10, 30$ MPa	For DEM model establishment and validation
Case 2	Veined granite	8	$\mu = 0$ (PC)	$\sigma_3 = 0, 3, 10, 30$ MPa	Rupture of veined rock under PC
Case 3	Veined granite	8	$\mu = -0.8, -0.5, 0.5, 0.8$ (PC)	$\sigma_3 = 10$ MPa	Role of σ_2
Case 4	Veined granite	16	$\mu = 0$ (PC)	$\sigma_3 = 10$ MPa	Effects of vein thickness and orientation ^b

Abbreviations: DEM = discrete element method; PC = polyaxial compression; TC = triaxial compression; TT = triaxial extension.

^aFor each σ_3 , σ_2 was varied with σ_1 to maintain a constant Lode parameter (equation (1)). ^bFour different thickness values ($t = 8, 12, 16$, and 20 mm) and four inclination angles ($\beta = 15^\circ, 30^\circ, 60^\circ$, and 75°) of the inclined vein (striking at σ_2 , Figure 2a) were considered in the simulation.

2.5.2. Veined Granite (Cases 2–4)

Three numerical scenarios were investigated for the veined granite; all numerical tests in the three scenarios were conducted in PC (Table 1). Note that for each case, simulations were performed on both soft-veined and hard-veined models to explore the difference of the rupture characteristics. The three scenarios are described below.

1. In case 2, the Lode parameter was set to be constant ($\mu = 0$), while σ_3 was set at 0, 3, 10, and 30 MPa; σ_2 increased against σ_1 to maintain a constant μ (equation (1)). As mentioned earlier, in each simulation σ_3 remained constant, and σ_2 was applied via the servomechanism in PFC 3D, and its value was updated cycle-by-cycle following equation (1) (note that the servomechanism in PFC 3D is a function, which can be used to apply a desired force on rigid walls, see PFC3D manual, 2008 for more details).
2. In case 3, a constant σ_3 of 10 MPa was set in the PC, while the Lode parameter was varied ($\mu = -0.8, -0.5, 0.5$, and 0.8) to study the effect of intermediate principal stress on the rupture of veined granite.
3. In case 4, 16 simulations were performed to study the effect of vein thickness and vein orientation on the rupture of veined rocks. In these simulations, both σ_3 and the Lode parameter were constant ($\sigma_3 = 10$ MPa; $\mu = 0$). Four different thickness values ($t = 8, 12, 16$, and 20 mm) and four inclination angles ($\beta = 15^\circ, 30^\circ, 60^\circ$, and 75°) of the inclined vein were considered.

2.5.3. Post Processing

ParaView 5.6.1 (<https://www.paraview.org/>) is used in the post processing for graphing and visualization. It is worthy to note that each rupture pattern shown in the results corresponds to the end of each simulation (at the time when vertical stress decreases to 80% $\sigma_{1, \text{peak}}$). The stress state at the point of model rupture is also reported.

3. Results

3.1. Granite Without Veins (Case 1)

3.1.1. Rupture Pattern

A total of twenty simulations were performed on the cubic BT granite models without veins. As shown in Figure 3, the mechanically induced cracks (shown as points in the figure) were plotted against computational time (i.e., cycle) in the 3D domain ($60 \times 60 \times 120$ mm) to show the fracture initiation, propagation, and rupture pattern (Figure 3). The three principal stresses at the time of model rupture are also shown in Figure 3. For clarity, the failure mode (tension or shear) of the cracks (bonds) was not shown in the figure. Under zero confinement ($\sigma_2 = \sigma_3 = 0$ MPa), cracks were induced at the opposite corners in the model, propagating from the model edge (blue cracks) to the middle (red cracks), and finally forming two macrofailure planes (Figure 3a, $\mu = 1$). When σ_2 was increased (Figure 3a, $-1 < \mu < 1$), clear shear bands were generated within the models in PC. These shear bands initiated approximately at the bottom edges of the models and then propagated and coalesced in the middle. The shear bands unambiguously dip toward σ_3 , in a situation that is in accordance with experimental observations (Mogi, 1967; Haimson, 2006; Ma & Haimson, 2016). The shear band angles (i.e., the angle between shear band and σ_1) decreased with the increase in σ_2 (i.e., from 26° at $\sigma_2 = 56$ MPa to 21° at $\sigma_2 = 175.5$ MPa, Figure 3a), in a general trend, which is compatible with laboratory

Figure 3. Rupture patterns of intact Bukit Timah granite models in triaxial compression (first column), polyaxial compression (second fourth columns), and triaxial extension (last column). (a) $\sigma_3 = 0$ MPa, (b) $\sigma_3 = 3$ MPa, (c) $\sigma_3 = 10$ MPa, and (d) $\sigma_3 = 30$ MPa. The stress state (i.e., σ_1, peak , σ_2 , and σ_3) at the point of model rupture in each simulation is also shown in the figure. Note that all rupture patterns correspond to the end of simulations (at a point when the axial stress dropped to 80% σ_1, peak). Microcracks are plotted as different-colored points with computational time (i.e., cycle), which enables a better understanding and visualization of crack initiation, propagation, and coalescence, as well as rupture pattern.

Figure 4. Plot of octahedral shear stress (τ_{oct}) versus effective mean stress ($\sigma_{m,2}$) based on the results of the numerical simulations shown in Figure 3. A linear fit, following the Mogi's format, was achieved.

remained essentially constant ($\sim 30^\circ$, Figure 3b). Besides which, more subhorizontal tensile bands were induced in the TT (Figure 3b, $\mu = -1$) compared with that shown in Figure 3a ($\mu = -1$).

Conjugate shear bands were observed in a model in PC when σ_3 was increased to 10 MPa (Figure 3c, $\mu = 0.5$), which was in good agreement with that observed in a laboratory experiment (Ma et al., 2016). Under relatively high confinement (Figures 3c [10 MPa] and 3d [30 MPa]), the induced shear bands exhibited more curvature. The shear band angles in the models under the relatively high confinement also show a consistently reducing trend compared to those observed in models under low confinement (Figure 3a) (from 39° at $\sigma_2 = 87.4$ MPa to 31° at $\sigma_2 = 236.8$ MPa, Figure 3c; and from 42° at $\sigma_2 = 122.3$ MPa to 35° at $\sigma_2 = 315.8$ MPa, Figure 3d). Besides, many more scattered cracks were also induced within the models under the high confining stresses.

3.1.2. Prediction of $\sigma_{1, peak}$ and Validation of DEM Model

Following on from equations (2) and (3), the numerical results were plotted in the τ_{oct} - $\sigma_{m,2}$ diagram (Figure 4), which yielded a single monotonically rising fitting curve that can be described by

$$y = kx^n \quad (k = 3.8, \quad n = 0.69) \quad (8)$$

The above linear relation between τ_{oct} and $\sigma_{m,2}$ qualitatively matches Mogi's critical discovery in their relationship. Also, the values of the two fitted Mogi's constants ($k = 3.8$ and $n = 0.69$) based on this numerical work fall within their respective ranges ($k > 1.5$ and $n < 1.0$), originally discovered by Al-Ajmi and Zimmerman (2005) through analysing many high-quality TC test data on various rocks. It is noted that it only makes sense to compare the Mogi's constants for the same lithology (from the same geological formations), because even for the same rock type sampled from with different formations, can yield somewhat different mechanical and mineralogical properties, which will lead to the variation of the values of the Mogi's constants.

The predictions of the $\sigma_{1, peak}$ based on Mogi's criterion are shown in the $\sigma_{1, peak} - \sigma_2$ plot (Figure 5a), together with the numerical results (points). The systematic variation in $\sigma_{1, peak}$ observed in the DEM study matches with the trend predicted by the Mogi's criterion (Mogi, 1971). It must be acknowledged that this well-correlated agreement relies on Mogi's constants (Figure 4), which in this study were determined based on numerical data rather than independent experimental data.

The modified Lade criterion was further used to analyse the $\sigma_{1, peak}$ of the intact BT granite in PC. In the study, the cohesion and friction angle of the fresh granite were 21 MPa and 50° (Zhou & Zhao, 2018), respectively. The two material constants, S_a and η , in the criterion described by equations (6) and (7) therefore can be calculated, which were 17.6 and 88, respectively. The $\sigma_{1, peak}$ values estimated by the modified Lade criterion were expected to reflect the real stress conditions at the time of model rupture. Figure 5b shows a

Figure 5. Comparison of the numerical data of the polyaxial tests on the intact Bukit Timah granite models and corresponding predictions from two well-recognized failure criteria, (a) Mogi criterion (1971) and (b) modified Lade criterion (1999).

comparison of the results from the DEM study, as well as those from the modified Lade criterion. Under relatively low confinement, the numerical results were in acceptable agreement with the corresponding predictions from the failure criteria, especially for the six tests in PC. However, clear discrepancies between numerical and empirical results were observed for the tests under somewhat higher confinement (30 MPa). This phenomenon is mainly due to the intrinsic limitation of the parallel bond contact model, which cannot provide enough interlocking such as occurring with natural mineral grains, especially under high confinement (Shang, Duan, et al., 2018; Zhang et al., 2019). Despite the limitation of this approach, it is still attractive because it can reproduce many significant physical features and mechanical mechanisms that occur in rocks, such as fracturing process, dilation, time-dependent behavior, and strength increase with confinement (Lee & Jeon, 2011; LongJohn et al., 2018; Potyondy & Cundall, 2004; Potyondy, 2007; Shang, Zhao, et al., 2018; Virgo et al., 2013; Zhang et al., 2019). The study based on the particle-based DEM approach can still provide us with some new insights into the rupture characteristics of veined rocks under in situ confinement, which has not been extensively emphasized before. In the following three cases, confining stresses no larger than 30 MPa were applied on the veined granite models.

3.2. Rupture of Veined Granite in Polyaxial Compression (Case 2)

3.2.1. Granite With Soft Veins

Four polyaxial compression simulations were performed on the BT granite containing soft veins (Table 1, case 2). In each simulation, σ_2 was varied against σ_1 to maintain a constant Lode parameter ($\mu = 0$). Four different levels of σ_2 were considered. Figure 6a shows the differential stress ($\sigma_1 - \sigma_3$) versus strain curves of the four models under different PCs; the strain of the models was differentiated in three components ($\varepsilon_1, \varepsilon_2, \varepsilon_3$) and plotted with different line shapes in the figure. The relations between $\sigma_1 - \sigma_3$ and volumetric strain, $\Delta V/V$ ($\Delta V = \varepsilon_1 + \varepsilon_2 + \varepsilon_3$), are also plotted (Figure 6b). The rupture pattern of the four models in PC are shown in Figure 7a, together with the presentation of the corresponding particle displacement field of the models, expressed at microscale in the x - and z -directions, respectively (Figures 7b and 7c).

As shown in Figure 6a, the peak of the differential stress $\sigma_1 - \sigma_3$ increased consistently from 51 ($\sigma_3 = 0$ MPa, $\sigma_2 = 25.5$ MPa) to 223.5 MPa ($\sigma_3 = 30$ MPa, $\sigma_2 = 141.6$ MPa). Under relatively low confinement ($\sigma_3 = 0$ and 3 MPa), the post-peak stress of the soft-veined granite dropped abruptly at the model rupture (red and black line in Figure 6a), exhibiting brittle failure. A gradual decrease in strain at relatively constant differential stress was observed for the model deformed at $\sigma_3 = 10$ MPa (green dotted line in Figure 6a). It is suspected that this gradually decreasing strain was caused by shear sliding and dilation, due to cracking of the soft veins (Figures 7a and 7b, $\sigma_3 = 10$ MPa). The sliding and dilation, however, were suppressed, and the soft-veined model was compacted at $\sigma_3 = 30$ MPa (Figures 6, blue line). The compaction of the soft veins can be reflected in the particle displacement field (Figure 7c, $\sigma_3 = 30$ MPa), where a clear horizontal isolation layer (i.e., a horizontal interface between cyan and green) can be observed. This clear difference in the displacement of the particles around the cracked horizontal vein implied that the horizontal vein was compacted. Perhaps this is why the strain line in Figure 6a (blue dotted line) did not flatten out (compared with green dotted line), as compaction of the horizontal vein reduced sliding along the inclined vein.

Figure 6. Differential stress ($\sigma_1 - \sigma_3$) against axial strain ($\epsilon_1, \epsilon_2, \epsilon_3$) (a) and volumetric strain ($\Delta V/V$ [$\Delta V = \epsilon_1 + \epsilon_2 + \epsilon_3$]) (b) for soft-veined Bukit Timah granite in polyaxial compression.

Although it is acknowledged that such inelastic compaction is often absent in intact granite (with very low porosity) (Yoon et al., 2012), similar stress-dependent dilation and compaction were also observed in laboratory experiments and reported by Turichshev and Hadjigeorgiou (2016) in veined andesite and by Ma et al. (2016) in porous sandstones. This is probably due to the compaction of broken veins (for soft-veined rocks) or the collapse of pores (for porous rocks).

Rupture of the soft-veined granite shows a clear confinement dependency. Model rupture often occurred along the inclined veins ($\beta = 45^\circ$) at $\sigma_3 = 0$ and 3 MPa (Figure 7a); a combination fracture of soft veins was observed when σ_3 was increased to 10 and 30 MPa. More interestingly, under relatively high confinement (Figure 7a [$\sigma_3 = 10$ and 30 MPa]), the rupture of the soft-veined granite occurred progressively. When $\sigma_3 = 10$ MPa, the onset of fracturing initially happened along the inclined vein, and a partial fracture of the horizontal vein was subsequently noticed, followed by the incomplete and progressive fracture of the vertical vein (striking at σ_2). A consistent fracturing process was observed when σ_3 was increased to 30 MPa (Figure 7a); however, in this case all the soft veins, except the one striking at σ_3 , were fractured. Additionally, many cracks were also noticed in the granite matrix (red in Figure 7a, $\sigma_3 = 30$ MPa) after the model rupture since the polyaxial compression continued under the high confinement until the vertical stress dropped to $80\% \sigma_{1, \text{peak}}$.

Another interesting point observed in the simulation (Figure 7a) was that only the inclined soft veins striking at σ_3 remained unbroken in the PC, although noticeable microcracks were induced in the veins. This is probably because σ_2 restrained the opening of cracks along its direction. This phenomenon has also been observed in the fracturing of stressed rocks, such as reservoir stimulation (Legartha et al., 2005; Stanchits et al., 2015).

The particle displacement field for each simulation shown in Figures 7b and 7c demonstrates a consistent trend of model deformation, although the magnitude of particle displacement was somewhat different (shown as a different color) due to the different stress conditions. The shear bands along the inclined veins were generated without exception, and the particles located on the top of the bands exhibited negative displacement in both σ_3 and σ_1 directions, while the particles at the bottom all yielded positive displacement, indicating that the soft-veined models were dominantly ruptured by shearing along the inclined veins in PC.

3.2.2. Granite With Hard Veins

To consider the effect of vein strength on rupture characteristics, BT granite models containing hard veins (i.e., quartz) were considered. Likewise, the hard-veined granite models were tested in PC with the same stress path applied on the soft-veined models (Table 1, case 2). It is found that all tested granite models containing hard veins ruptured in brittle mode (Figure 8). One model yields a clear axial strain (Figure 8a, black dotted line), which was not due to the sliding failure of the model (as that observed in Figure 6a, green dotted line) but as a result of local rupture of the hard-veined granite (see Figure 9a, $\sigma_3 = 0$ MPa). This was further verified by its corresponding particle displacement field (Figures 9b, $\sigma_3 = 0$ MPa), where no excessive shear sliding was observed as that observed in soft-veined models (Figure 7b). It is suspected that the energy within the hard-veined brittle granite under zero σ_3 confinement was released suddenly along σ_3 due to the high axial loading ($\sigma_1 = 245.5$ MPa) and low confinement ($\sigma_3 = 0$ MPa).

Figure 7. Rupture pattern of soft-veined Bukit Timah granite in polyaxial compression (a), and particle displacement field in the σ_3 (b) and σ_1 (c) directions (the unit of stress is MPa).

Conjugate shear bands were observed for two cases (Figure 9a, $\sigma_3 = 3$ and 10 MPa), where the hard-veined models all ruptured within the rock matrix and the hard veins impeded localized rupture along the veins. The corresponding displacement field of the two cases (Figures 9b and 9c [$\sigma_3 = 3$ and 10 MPa]) show their deformation characteristics, where the displacement field was roughly divided into four parts (coded in color) by the conjugate shear bands. When σ_3 was increased to 30 MPa (Figure 9a), the main shear band that was subparallel to the inclined hard vein was observed in the model.

Compared with the soft-veined granite, the hard-veined granite in PC exhibited much higher $\sigma_{1, \text{peak}}$ (although this can be anticipated) and brittleness. Their rupture patterns were also fundamentally different compared with that of soft-veined models and were not controlled by the hard veins.

Figure 8. Plot of σ_1 - σ_3 and axial strain (a) and volumetric strain (b) for the hard-veined Bukit Timah granite models in polyaxial compression (the unit of stress is MPa).

3.3. Role of σ_2 (Case 3)

A further investigation focused on the σ_2 effect, which has long been recognized and was originally reported by Mogi (1967). As shown in Table 1 (case 3), four Lode parameters ($\mu = -0.8, -0.5, 0.5$, and 0.8) were selected in PC, and σ_3 remained constant (10 MPa) in each case, σ_2 being varied against σ_1 to maintain a constant μ in each simulation. A total of eight simulations were performed, including four on soft-veined models and four on hard-veined models.

3.3.1. Rupture Characteristics

Overall, σ_2 has a significant influence on the rupture characteristics of the veined granite, irrespective of vein mechanical strength. The soft-veined granite models show a consistent shear rupture characteristic along the inclined veins, which occurred within the cycle of 120,000 (blue or light cyan cracks in Figure 10a). The shear rupture planes can also be demonstrated by the displacement field in the σ_3 direction (Figure 10b).

Following the fracture of the inclined veins, the subsequent rupture of the four soft-veined models exhibited somewhat discrepancies. For $\mu = 0.8$ (Figure 10a), the horizontal vein was fractured, approximately in conjunction with the partial fracturing of the top areas of the vertical vein (striking at σ_2); at the latter stage of the simulation (after cycle of 151,811), many microcracks, shown as orange and red, can be observed within the rock matrix, which was probably due to stress concentration. A quite similar rupture characteristic was observed at $\mu = 0.5$ (Figure 10a). However, when the value of μ fell between -0.5 and -0.8 , the vertical veins striking at σ_2 were almost fractured, which was mainly due to the apparently much higher σ_2 and was according with many more microcracks induced within the vertical veins striking at σ_3 . This phenomenon, however, was not observed in the other two cases (Figure 10a, $\mu = 0.5$ and 0.8).

The rupture of the four hard-veined granite models shows somewhat similarity (Figure 10b), in terms of the formation of conjugate shear bands. Compared with the soft-veined granite, the rupture of the hard-veined granite was not localized by the vein structures, especially for the two cases under high σ_2 (Figure 10b, $\mu = -0.5$ and -0.8).

3.3.2. Effect of σ_2 on $\sigma_{1, \text{peak}}$ and Deformability

As seen in Figure 10a, under constant σ_3 (10 MPa), a continuous increase in $\sigma_{1, \text{peak}}$ (from 108.8 to 143.1 MPa) with increasing σ_2 was observed for the soft-veined granite, which is not in accordance with the evolution trend of $\sigma_{1, \text{peak}}$ due to the σ_2 effect, as that observed in the intact BT granite (Figure 5). It is suspected that this was probably because of the inelastic behavior of the soft veins, which significantly affected the rupture patterns of the veined rock, and these veins were fractured continuously with an increase of σ_2 (Figure 10a). While for the hard-veined granite, which behaves more like that of intact rock in PC (Figure 10b), $\sigma_{1, \text{peak}}$ increased from 306.3 MPa (at $\sigma_2 = 39.6$ MPa) to a maximum value (i.e., 327 MPa, at $\sigma_2 = 248.8$ MPa) and then reduced to 317.5 MPa when σ_2 was furthered increased (to 286.8 MPa). This $\sigma_{1, \text{peak}}$ evolution trend, because of σ_2 , agrees well with that observed in intact rocks (Mogi, 1967; Ma et al., 2016).

The effect of σ_2 on the deformation characteristics was examined by plotting σ_1 - σ_3 versus axial strain and volumetric strain curves of soft-veined (Figures 11a and 11b) and hard-veined (Figures 11c and 11d) granite models. Similar to that observed in Figure 6a, gradual increases in axial strain at relatively constant

Figure 9. Rupture pattern of the hard-veined Bukit Timah granite models in polyaxial compression (a), and particle displacement field in σ_3 (b) and σ_1 (c) directions (the unit of stress is MPa).

differential stress were observed for the soft-veined models under relatively low confinement (black and green dotted lines in Figure 11a), which was probably associated with the shear sliding along the fractured soft veins. However, the shear slide deformation, along soft inclined veins, was suppressed when σ_2 was increased to 104.2 and 130 MPa, respectively (Figures 11a and 11b, red and purple lines). Hard-veined models exhibited much brittle failure (Figures 11c and 11d), without showing the shear sliding behavior observed in soft-veined models.

3.4. Impact of Vein Orientation and Thickness on Rupture Behavior (Case 4)

This section reports the results of an examination of the impact of vein orientation and thickness on the rupture characteristics of both soft- and hard-veined granite (Table 1, case 4). For simplicity, only the inclined

Figure 10. Effect of σ_2 on the rupture characteristics and particle displacement field of the soft-veined Bukit Timah granite models (a) and hard-veined Bukit Timah granite models (b) in polyaxial compression. σ_3 remained constant (10 MPa) in each simulation, and σ_2 was varied against σ_1 consistently to maintain a constant Lode parameter (the unit of stress is MPa).

Figure 11. $\sigma_1 - \sigma_3$ against axial strain for the soft-veined granite models (a) and hard-veined granite models (c). $\sigma_1 - \sigma_3$ against volumetric strain for the soft-veined granite models (b) and hard-veined granite models (d).

vein geometry (i.e., thickness and orientation) was varied in the study because the inclined vein plays the most important role that can affect the mechanical behavior of veined rocks (Turichshev & Hadjigeorgiou, 2015, 2017).

The thickness of a vein in nature can vary from a millimeter scale to centimeter (Figure 1), and the values of vein thickness generally follows a power law distribution (André-Mayer & Sausse, 2007). Considering the dimension of the model, in this work four vein thicknesses (Figure 12a [$t = 8, 12, 16$, and 20 mm]) were assigned to the inclined vein (β was constant, $=45^\circ$); four vein inclinations relative to horizontal (in the x -positive direction) were selected (Figure 13a [$\beta = 15^\circ, 30^\circ, 60^\circ$, and 75°]), where t was constant ($=5$ mm) in this series of simulations. A total of 16 simulations were performed considering both hard and soft veins for each vein thickness and inclination. The numerical results in terms of fracture initiation, propagation, final rupture pattern, and the stress state at the point of model rupture were interpreted and shown in Figures 12 and 13.

The influence of vein thickness on the mechanical behavior of both soft- and hard-veined granite was not pronounced (Figures 12b and 12c), which is in good agreement with the observation in a laboratory study (Turichshev & Hadjigeorgiou, 2017). The rupture pattern of the four soft-veined granite models shows high similarity in shape, except for the thickness of the shear bands (Figure 12b). A slight increase in $\sigma_{1, \text{peak}}$ (within 18%) was observed when the thickness of the soft vein reduced from 20 to 8 mm. While a much smaller increase in rate (from 340.6 to 343.2 MPa, 0.8%, Figure 12c) for $\sigma_{1, \text{peak}}$ was observed in the study for the hard-veined models when the vein thickness was reduced.

On the contrary, vein orientation significantly affected the rupture characteristics of all tested models, especially for those containing soft veins (Figure 13b). As seen in Figure 13b (at $\beta = 75^\circ$), the soft-veined model ruptured firstly along the high-inclined vein; the horizontal vein was also fractured to some degree. One more interesting point observed was that, in the latter stage of the simulation (after cycle of 134,931), many microcracks (red in Figure 13b, $\beta = 75^\circ$) were induced and clustered at areas close to the two ends of the

Figure 12. (a) Setup of models with different thicknesses of veins. Only the inclined vein thickness was changed ($t = 8, 12, 16$ and 20 mm), other setup conditions are the same as that shown in Figure 2a. Influence of vein thickness on the rupture characteristics of the soft-veined granite models (b) and hard-veined granite models (c) (the unit of stress is MPa).

inclined vein. This was probably due to stress concentration at those areas around the fractured vein, as the numerical test continued after the model rupture until the vertical stress dropped at $80\%\sigma_{1,peak}$. The stress concentration-induced fracture disappeared when β was reduced to 60° (Figure 13b), where only one major shear band along the inclined vein was produced. Much more complex rupture patterns were observed at $\beta = 30^\circ$ and 15° (Figure 13b); all soft veins, except the one striking at σ_3 , were fractured within the cycle of

Figure 13. (a) Setup of models with different orientations of veins ($\beta = 15^\circ, 30^\circ, 60^\circ$, and 75°). Influence of vein orientation on the rupture characteristics of the soft-veined granite models (b) and hard-veined granite models (c) (the unit of stress is MPa).

287,321, and after which many microcracks were induced within the rock matrix (shown as orange/red). The magnitude of $\sigma_{1, peak}$ was also varied significantly for the four soft-veined models, which reduced from 120 MPa at $\beta = 75^\circ$ (Figure 13b) to 90 MPa at $\beta = 60^\circ$ and finally increased dramatically to 243.5 MPa at $\beta = 15^\circ$.

The variation of $\sigma_{1, \text{peak}}$ for the four hard-veined models was not remarkable compared with that of the soft-veined models, which was basically within 2.7% (maximum = 350.7 MPa, minimum = 341.6 MPa, Figure 13c). Conjugate shear bands were observed at $\beta = 15^\circ$ (Figure 13c), and a similar shear rupture pattern was noted for the other three cases ($\beta = 30^\circ$, 60° , and 70°).

4. Discussion

4.1. Model Simplification and Assumption

4.1.1. Vein Strength and Geometry

Veins, formed naturally from mineral precipitation in a fluid within fractures, are almost ubiquitous in the upper crustal rocks and can be easily distinguished by eye in the field due to the distinct color contrast between vein-filling minerals and their host rocks (Figure 1). The hardness can be used to estimate the strength (e.g., UCS) of homogeneous vein-filling minerals (Grigg, 2016). Several experimental studies have demonstrated that hardness is linearly correlated with the yield strength and UCS of brittle, crystalline materials (Aliyu et al., 2019; Hucka & Das, 1974; ISRM, 1981; Kahraman et al., 2012; Zhang et al., 2011). It is noted that the yield strength of brittle, crystalline materials is approximately equal to the uniaxial tensile strength (Zhang et al., 2011). One common hard vein-filling mineral appeared in granite is quartz, which is one of the most common minerals in the Earth's crust and has a Vickers hardness (H_V) of $\sim 1,161 \text{ kg/mm}^2$. Other relatively softer vein-filling minerals like calcite ($H_V = 157 \text{ kg/mm}^2$) and gypsum ($H_V = 61 \text{ kg/mm}^2$) are also quite common in nature, which tend to weaken the overall strength of veined rocks (Day et al., 2019).

In this study, it is assumed that the mechanical properties (e.g., UCS, stiffness, etc.) for an individual vein in the core-scale models (Figures 1 and 2) were isotropic, although in nature these properties, especially at the field scale, can be anisotropic (Day & Clark, 2019; Laubach et al., 2004), resulting from imperfect cementation, tectonic activities, or rotation of in situ stresses (Gomez-Rivas et al., 2014; Holland & Urai, 2010). This isotropy assumption follows that used in Sone and Zoback (2013) and in many other numerical and analytical studies that focused on the failure of anisotropic rocks containing strong and weak layers rather than veins (e.g., Bourne, 2003; Na et al., 2017; Shang, Duan, et al., 2018; Shang et al., 2019; Yin & Yang, 2019), where the layers were assumed to be isotropic and distinguished either by mechanical properties (e.g., tensile strength) or by stiffness (e.g., Young's modulus).

Since there is no known knowledge of the hardness values of the quartz and calcite within the BT granite, to simplify the problem, I use the standardized hardness values of both quartz, calcite, and granite in literature in the microparameter calibration. I anticipate that this practice can lead to a more reliable strength ratio between veins and granite matrix in this computational study, which benefits the current research on the vein-granite interactions and model rupture. I acknowledge that this simplification may lead to a non-negligible discrepancy, but it is expected within an acceptable range because the average UCS of the granite reported in the literature is $\sim 200 \text{ MPa}$ (Hasirci & Hasirci, 2018; Lewis et al., 2003), which is close to that of BT granite in this study (186 MPa).

For simplicity, the calcite-granite interface has the same strength as that of granite; the quartz-granite interface has the same strength as that of quartz. This scheme allows the overall rupture characteristics of the veined models to be focused (which is the main objective of this research) by simplifying the interface fracture problems (Virgo et al., 2013).

The geometry and internal structure of veins can vary as a result of different mineral precipitation rates, various fracture geometries, as well as tectonics (Bons et al., 2012). For simplicity, the DEM model shown in the study (Figure 2a) was established with a priori vein geometry to correspond to a natural prototype of BT granite (Singapore) that contains authigenic cement (Figure 1d).

4.1.2. Model Resolution and Particle Packing

In this study, a uniform particle size distribution ($r_{\text{max}}/r_{\text{min}} = 1.66$, $r_{\text{min}} = 0.6 \text{ mm}$) was used to establish the DEM model, which follows the scheme used in Shang, Duan, et al. (2018). I have not attempted to reproduce the real mineral grains of granite but attempted to establish a model that can mimic the mechanical behavior of the rock. Each model contains a total number of 133,871 particles (Figure 2a), which is enough to capture the failure mechanism of real rocks (Potyondy & Cundall, 2004), considering the size of the model ($60 \times 60 \times 120 \text{ mm}$). As seen in the preliminary study (case 1 in Table 1), the established DEM model yielded a plausible rupture feature in PC (Figures 3 and 4), which was comparable with previous findings (Mogi, 1967; Pan

et al., 2012, Ma et al., 2016) and predictions from failure criteria (Figure 5). This gave much confidence of the selection of the model resolution and of the application of the model to investigate the rupture characteristics of veined granite in PC.

In addition, the models used in the study were developed using the random particle packing approach (PFC 3D manual, 2008). A constant seed (100,00) for a random-number generator was used to generate identical models, although the strength within a random particle packing may not be ideally homogeneous (Koyama & Jing, 2007). The macroscopic strength contrast between the veins and bulk material in the DEM models in the study mainly arises from a combination of two components: (1) the (known, prescribed) difference in bond strength parameters and (2) the (unknown) strength difference due to heterogeneities introduced by the particle packing. The vein width of most models shown in the paper is as small as 3–4 particles (5-mm vein thickness, cases 1–3) that can minimize the strength difference arising from particle packing, although it has been observed that a significant variation of strength between different particle packings exists, sometimes excess of 10% for samples with a ~10-particles wide (Koyama & Jing, 2007). Also, the strength contrast between the bulk and the vein materials, based on the bond parameters, is at least 37% (e.g., quartz/granite = 1.37), which will likely not have an impact on the qualitative results obtained. However, quantitative results based on this setup may acknowledge the uncertainty from particle packing.

4.2. Comparison of Results With Previous Findings and Implications of the Study

The results of the present study show that the soft veins localized rupture along veins (Figures 7, 10a, 12b, and 13b), while the hard veins enhanced the overall mechanical properties of the rock and impeded localized rupture (Figures 9, 10b, 10c, and 13c), which is in accordance with Virgo et al. (2013) and Vass et al. (2014). A gradual decrease in strain at relatively constant differential stress was observed in a soft-veined model (green dotted line in Figure 6a), which was probably due to the fracturing of the inclined soft vein, leading to shear sliding. The sliding and dilation, however, was restrained when the confinement was increased (Figure 6b, blue line), which complements the experimental data reported by Turichshev and Hadjigeorgiou (2016) and Ma et al. (2016).

The rupture of the soft-veined granite was highly dependent on confinement (Figure 7a). Low confinement ($\sigma_3 < 10$ MPa and $\sigma_2 < 67$ MPa in the study) led to the formation of localized rupture planes along weak veins, while high confinement resulted in a combination failure of the soft veins and the rock matrix. This, of course, can be anticipated but has rarely been justified in experiment because of the practical difficulty in the setup of PC tests on natural-veined rocks.

The study also shows that the veins striking at σ_3 in the soft-veined models remained unbroken in PC (Figures 7a and 10a), probably due to the suppression of σ_2 , which is in good accordance with previous observations on the fracture pattern of stressed rocks (Legartha et al., 2005; Stanchits et al., 2015).

Conjugate shear bands were generated in the hard-veined models (Figure 9) in PC; similar observations were also made in laboratory experiments on intact rocks (Artkhonghan et al., 2018; Crawford et al., 1995; Ma et al., 2016).

Many studies reveal that $\sigma_{1, \text{peak}}$ varies consistently against σ_2 for a particular σ_3 , which is often termed as the σ_2 effect (Haimson, 2006; Mogi, 1967). The σ_2 effect was also observed in the PC tests on the intact models (Figures 3 and 5) and the hard-veined models (Figure 10b). However, a continuous increase in $\sigma_{1, \text{peak}}$ was observed for the soft-veined models when σ_2 was increased (Figure 10a). This was probably associated with the inelastic behavior of the soft veins (Alejano & Alonso, 2005; Mura, 1987), which dominantly controlled the rupture feature of the soft-veined models.

This study also demonstrated that vein thickness had a negligible impact on the rupture characteristics of the veined models (Figure 12), irrespective of the vein strength. Vein orientation, on the contrary, exhibited a profound influence (Figure 13) on the rupture of the veined models, which was also observed in a laboratory test by Turichshev and Hadjigeorgiou (2017).

The above new insights gained from this 3D DEM study provide an in depth understanding of the integrity and rupture characteristics of veined rocks under in situ stress conditions. It have been numerically demonstrated that it is crucial to assess the strength contrast of host granite and veins (if present), as well as vein

orientation relative to in situ stress conditions, in the subsurface energy-related activities such as long-term disposal of high-level radioactive waste in granite repositories several hundreds of meters below the surface of the Earth and for underground storage of oil and gas in unlined granite caverns.

5. Conclusion

This study presents new insights into the rupture characteristics of veined granite under true triaxial stress regimes in detail. The aim was achieved by establishing a three-dimensional DEM model with a priori vein structure that corresponds to a natural prototype of veined Bukit Timah granite, which was collected in a borehole drilled up to ~200 m below the surface of the Earth in Gali Batu, Singapore. A novel stress path was applied in the PC, where σ_3 remained constant in each numerical test; σ_2 was varied against σ_1 to maintain a constant Lode parameter. Four numerical scenarios with fifty-two DEM simulations (Table 1) were analysed to examine the rupture characteristics of veined granite in PC, considering various factors including stress path, vein mineralogy (in terms of mechanical strength), and vein geometry (thickness and orientation). The results of the numerical study have been compared and validated against previous experimental findings and empirical predictions. The following points are concluded from this work:

1. Veins exhibited a pronounced effect on the rupture characteristics of Bukit Timah granite. Soft veins localized rupture along veins, while hard veins impeded localized rupture and enhanced the overall mechanical strength of the veined granite.
2. For the soft-veined models, rupture occurred along the inclined veins (45° relative to the horizontal with strike running in the σ_2 direction) under low σ_2 (<67 MPa in the study); in contrast, a combination rupture of veins and rock matrix appeared when σ_2 was increased to 141.6 MPa.
3. A gradual decrease in strain at relatively constant differential stress was observed for the model deformed at $\sigma_3 = 10$ MPa (green dotted line in Figure 6a), which was probably due to shear-induced volumetric dilation along the fractured vein. The sliding and dilation were restrained when σ_3 was increased to 30 MPa, which was perhaps due to the compaction of the horizontal vein under the relatively high confining stresses (which can be observed in the displacement field).
4. Compared with the soft-veined granite, the hard-veined granite in PC exhibited much higher $\sigma_{1, \text{peak}}$ (although this can be anticipated) and brittleness. Clear displacement of particles along σ_3 was observed for the hard-veined models under high $\sigma_{1, \text{peak}}$ (245.5 MPa) and low σ_3 (0 MPa).
5. Conjugate shear bands were generated in the hard-veined models in PC, similar to that formed in intact rocks.
6. The σ_2 effect, in terms of the consistent evolution in $\sigma_{1, \text{peak}}$ against the variation of σ_2 under a constant σ_3 , was also observed in the hard-veined models. However, a continuous increase in $\sigma_{1, \text{peak}}$ was observed for the soft-veined models when σ_2 was increased, which was probably due to the inelastic behavior of the soft veins.
7. Vein thickness had a negligible effect on the rupture characteristics, which was however profoundly affected by vein orientation, relative to the stress field.

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