PFC simulation of crack evolution and energy conversion during basalt failure process

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Abstract
Rock failure is an important phenomenon associated with crack propagation and energy conversion. In this paper, the uniaxial compression test of basalt is performed and acoustic emission (AE) activity is monitored throughout the process. The fracture characteristics and evolution of an internal crack in basalt are analyzed in detail with the obtained experimental data. A parallel bonding model is proposed in this study to investigate the failure of basalt subjected to uniaxial compression. The microscopic properties of particles and bonds in the model are calibrated against the results of mechanical behavior measured through physical experiments. We investigated the crack types and statistics of crack number by using a fish program in Particle Flow Code (PFC) under uniaxial compression. Meanwhile, the discrete element computational model monitored the information of energy upon each bond breakage during the loading process. All the numerical and test results are presented in graphs and discussed in detail. The PFC can accurately reproduce the crack propagation, failure patterns and energy conversion of basalt on a microscopic scale, which may not be monitored in the actual test.

Keywords: basalt, failure, crack evolution, energy conversion, particle flow code

1. Introduction
Rocks are used as major geological body, and their mechanical behaviors such as deformation, damage and fracture are extremely important in developing engineering endeavors and understanding geological processes (Main et al. 2000; Heap et al. 2011). The research into rock failure and fracture processes is a basic problem of theoretical calculations and designs in undergrounding engineering (Lai et al. 2017). Furthermore, the intrinsic mechanism during the deformation and fracture of rocks can be disclosed by research into meso-damage mechanics. However, the failure mechanism of brittle rocks is limited by the complexity of environment, diversity of rock types and differences of analytical means. Quantitative understanding of this failure process is indispensable to design in engineering endeavors, which may provide a theoretical basis and reference for the evaluation of deformation and stability in rock engineering.

For a long time, scholars devoted great efforts to study the mechanical properties, constitutive relation, mechanical models and calculation methods of rock failure (Fairhurst & Cook 1966; Wawersik & Fairhurst 1970; Bobet & Einstein 1998; Sahouryeh et al. 2002). The research and understanding of rocks have developed from continuum mechanics to discrete mechanics of discontinuous media, homogeneous isotropic medium to heterogeneous anisotropic media, the macroscopic mechanical model to the exploring of micromechanical behavior, and have established the equivalent relationship between them. Current thinking suggests that the strength of brittle rocks under compression depends on the internal microscopic structure, especially when controlled by the evolution and accumulation of damage on the microscopic scale (Lockner 1993; Lan et al. 2010; Peng et al. 2017). Previous studies suggested that, with an increase of deformation, the formation of macrocracks is the
result of the coalescence and propagation of microcracks, which may also cause the strength and stiffness degradation of rock and eventually resulting in a structural failure (Manouchehrian & Cai 2016; Wu et al. 2017). With the tremendous development in the proficiency and power of numerical programs, the numerical analysis method is enjoying a boom and has been increasingly applied to study the macroscopic consequences of microscopic structure on deformation and strength in brittle rock (Mishra 2003; Hoek & Martin 2014; Fan et al. 2018). The method of numerical simulation is the fundamental way to further explain the damage mechanism and law during rock failure. In particular, many studies have suggested that the application of discrete element method could be more advantageous than classical numeric methods, such as finite element, finite differences and boundary elements, in understanding the microscopic mechanics of rock. In the discrete element method (DEM), both the microstructure of a rock and dynamics of the fracture can be better captured.

In view of the above, the DEM becomes one of the most efficient computational approaches to studying rock mechanical characteristics. In recent years, DEMs such as lattice, particle and granular dynamics models have developed and obtained many achievements (Evans & Murad 1977; Place & Mora 1999; Matsuda & Iwase 2002; Yao et al. 2017). The DEM has been successfully utilized to study rock fracture (Donze et al. 1997; Young et al. 2000; Boutt & Mcpherson 2002; Chang et al. 2002; Hunt et al. 2003), rock fragmentation (Liu et al. 2002; Su et al. 2009), crack propagation and coalescence (Camones et al. 2013; Haeri et al. 2014), acoustic emission (AE) activity (Hazzard et al. 2000; Khazaee et al. 2015), localization phenomena (Zhou & Zhang 2017), mechanical properties of jointed rock mass (Jiang et al. 2017; Wang et al. 2017; Regassa et al. 2018), rock cutting (Su & Akcin 2011; Van Wyk et al. 2014) and load-unload response (Yin et al. 2000; Wang et al. 2004). PFC (particle flow code) appears to be a more efficient method to study the variation of a microstructure, which can provide an important reference for the macroscopic theory of rock, and is beneficial to understanding the essence of rock mechanical behaviors and engineering phenomena (see figure 1). However, these models place emphasis on the igneous rocks such as granites (Bäckström et al. 2008; Hofmann et al. 2015), sedimentary rocks such as marble (Liu et al. 2012; Huang et al. 2013) and sandstones (Yang et al. 2014; Kang et al. 2015) and coal (Zhao et al. 2015; Zhang et al. 2017), but only very few studies have tried to simulate the basic igneous rocks such as basalt.

The current research presents a 2D simulation procedure in order to study the behavior of basalt, in which crack propagation and energy evolution can be captured. First, the laboratory experiments were conducted on the cores. During the compressive tests, AE data was monitored to analyze the release and dissipation of energy. The macroscopic mechanical
properties and stress-strain curves of basalt were taken as the selection basis of microscopic parameters in PFC. The corresponding numerical model was established for a more profound understanding of the mechanical behavior of basalt. Both the experimental and numerical simulation provided an insight into how the cracks and energy evolve from micro to macro during the damage process.

2. Bonded particle models

The Particle Flow Code, PFC2D (Itasca 2014) was undertaken to simulate the uniaxial compression test. PFC modeling software is based on DEM, of which the basic mechanical properties of a material are described by the movement of each particle and the force and moment acting at each contact. In this model, rock is generally made up of a group of particles bonded together by parallel bonds (Potyondy & Cundall 2004; Park & Song 2009), similar to those observed microscopically in rock (Trent et al. 1987; Jirasek & Bazant 1993; Donzé & Magnier 1995). The strength of rock material is realized by the parallel bond between particles, and its essence is the cementing effect between particles (Bieniawski 1967; Bobet & Einstein 1998; Thompson et al. 2006).

The linear parallel-bond model is comprised of two interfaces (see figure 2), the first is an infinitesimal, linear elastic and frictional interface, which does not resist relative rotation and sliding. The other one is called a parallel bond, which is a finite-size, linear elastic and bonded interface, transmits a force and moment and can undertake the elongation, compression, shear and torsion of the interaction particles (Itasca 2014). The behavior of the parallel bond is linear elastic before reaching the strength limit of bonds. When the bond breaks, it is removed from the system and can no longer resist relative rotation at the contact.

The inter-granular viscous interaction is provided by parallel bonding, and the mechanical properties of particle are determined by the random microstructure of particle by transforming the torque into stress to realize rotational impedance. The parallel-bond force consists of normal force and shear force, and the parallel-bond moment is resolved into a twisting and bending moment:

\[ F_c = F^l + F^d + F_i \]
\[ M_c = \bar{M}_c \]
\[ F = -F_n n_c + F_s \]
\[ \bar{M} = \bar{M}_c n_c + \bar{M}_t \]

where \( F^l \) is the linear force, \( F^d \) is the dashpot force, \( \bar{M} \) is the parallel-bond force and \( \bar{M}_c \) is the parallel-bond moment.

Bonds break when they get overstressed during the evolution of the system, the breaking of a bond is mainly caused by stretching and bending:

\[ \bar{\sigma} = \frac{\bar{F}_n}{A} + \bar{\beta} \frac{\bar{M}_c \bar{R}}{I} \]
\[ \bar{\tau} = \frac{\bar{F}_s}{A} + \bar{\beta} \frac{|\bar{M}_t| \bar{R}}{J} \]

where \( \bar{F}_n, \bar{F}_s \) indicate the normal and tangential stress acted to contact and \( \bar{M}_c, \bar{M}_t \) are the bending moment and the twisting moment, respectively. \( \bar{\beta} \) is the moment-contribution factor, by default \( \bar{\beta} = 1 \). If \( \sigma_{\max} \geq \bar{\sigma} \) or \( \tau_{\max} \geq \bar{\tau} \) the cemented contact between particles breaks, where \( \bar{\sigma} \) and \( \bar{\tau} \) represent the tensile and shear strength of the cemented bond, respectively.
The fracture mechanism between particles; red indicates the tensile crack and blue indicates the shear crack.

The cross-sectional nature of the bond:
\[
\bar{R} = \bar{λ}_{\text{min}} \left( R^{(1)}, R^{(2)} \right),
\]
\[
\bar{A} = \pi \bar{R}^2,
\]
\[
\bar{I} = \frac{1}{4} \pi \bar{R}^4,
\]
\[
\bar{J} = \frac{1}{2} \pi \bar{R}^4.
\]

where \( \bar{A} \) is the area of the parallel-bond cross-section, \( \bar{I} \) and \( \bar{J} \) are the moment of inertia and polar moment of inertia on the parallel-bond cross-section, respectively.

The PFC software can record crack propagation through the embedded fish language. This simulation focuses on the mechanism of rock fracture from microcosmic point of view, and analyzes the deformation process from linear elastic stage to fracture failure. In order to deal with the formation and propagation of cracks directly, each bond of this model is assumed to break. There are two forms of crack, shear crack and tensile crack. When the shear strength of bond is exceeded, a shear crack is found; while when the normal strength of bond is exceeded, a tensile crack results (see figure 3). The formation of microcracks gives rise to the stress redistribution within a rock specimen and this then leads to the failure of rock by the formation of a shear-zone during compression tests.

### 3. Simulation of uniaxial compressive test

#### 3.1. Experimental set-up and numerical model

The material used throughout this study was obtained from a tunnel of Mount Emei China. The basalt was chiefly composed of crystals of feldspar (~34–45%), groundmass (~15–30%), crystals of pyroxene (~8–15%) and plagioclase (~3–5%). With the presence of these minerals, basalt owns its characteristic light gray color. Basalt possesses a compact structure, having a bulk density of 2750 kg m\(^{-3}\). Basalt shows complex mechanical properties such as discontinuity, non-uniformity and anisotropy, which are different from the continuous medium.

The rock specimens for uniaxial compressive tests were produced as cylindrical specimens with a \( \phi \) size of 50 \( \times \) 100 mm. Both ends of rock specimens were ground to burnished faces and thoroughly cleaned to ensure the parallel misalignment and non-perpendicularity within \( \pm 0.02 \) mm. The WAW-60 Electro hydraulic servo testing machine system was used for loading, while the AE21C system was applied to monitor the AE signals. The strain monitoring was carried out by using LVDT transducers until rock failure. Figure 4 shows the schematic diagram of the physical experiment. During uniaxial compression tests, the deformation and failure behavior of basalt samples were recorded concurrently with PC-based systems. At the same time, the AE signals could be monitored and recorded from initial loading to final failure of basalt.

PFC allows to simulate of the uniaxial compressive test with the size set to width \( D_0 \) and height \( H_0 \), where \( H_0/D_0 = 2 \) as in the uniaxial compressive tests (see figure 5). The pressure load, produced from the compression testing machine in uniaxial compressive tests, was utilized in the simulation. By way of simulating the mechanical behavior of rock more accurately, we had to calibrate the microscopic properties of the numerical model against the controlled laboratory experiment.

#### 3.2. Calibration of micro-scale parameters

In PFC, the macroscopic response of material is inferred from the interaction of the input microscopic properties. The aim of calibration of micro-scale parameters is to obtain the parameters of particles and bonds in the PFC calculation. Microscopic properties, such as contact stiffness and bond strength, are assigned as input parameters, which are usually unknown. The relationship between the input microscopic properties and target macroscopic parameter, such as Young’s modulus, Poisson ratio and UCS, are not directly related. The calibration process of PFC involved recognition of the main input parameters, sample generation and running plenty of numerical simulations by adjusting the main input microscopic parameters continuously until the desired macroscopic behavior was reproduced. According to physical experiments (see figure 6), the related microscopic parameters of model constituents in PFC were inverted to describe the mechanical properties of basalt. In this process, we needed to ensure that the stress-strain curve of numerical simulation was consistent with the experiment. Then, \( \sigma \) and E were calibrated. In the last step, the failure mode and the crack coalescence process of experimental and numerical simulation are compared, which can be relatively consistent.

The micro parameters used to reproduce the physical experiments with a PFC model are shown in Table 1. This
group of micro-scale parameters can accurately describe the macroscopic mechanical properties of basalt under uniaxial compression.

The stress-strain relationship of numerical simulation and a uniaxial compressive test are both shown in figure 7. According to the results, the shape of the curves is similar, the strength and stiffness of the basalt are approximately reproduced by the model.

As shown in figure 7, the most obvious difference between the numerical simulation and experiment is the lack of initial curvature observed during the laboratory tests at low stress levels. The absence of the curvature in the model response is due to the fact there are no preexisting fissures in the model, and it has not experienced a compaction process of pores and cracks. Stress of the experiment and numerical simulation dropped rapidly after reaching the peak strength, indicating brittle feature.
4. Discussion of rock failure

4.1. Microcrack propagation

To understand the inherent law of rock failure and the essential characteristics of fracture instability, it is necessary to start with the formation, growth and eventual interaction of microcracks in basalt. In the numerical simulation, the failure criterion is calculated at each iteration step of the system. When the bond between particles satisfies the failure condition, a crack will be created and the crack number is equal to the amount of broken bonds in the contact model. The change of contact relation between particles, such as disconnection, could affect the macroscopic mechanical properties of the medium.

From figure 8 we can see that the deformation and failure process of basalt under uniaxial compressive can be approximately divided into four phases: (1) closing of cracks in the laboratory test, while in the numerical model, this phase will not appear (see figure 8b), (2) the linear elastic region, (3) crack initiation and stable crack propagation and (4) crack coalescence and unstable crack propagation.

As shown in figure 8a, AE events indicate the propagation of microcracks in the basalt sample. The corresponding numerical result of microcracks growth in different phases by means of PFC2D is shown in figure 8b. In order to show the cracks location and evolution clearly, the display of the crack has been adjusted; the red mark represents the tensile crack and the blue mark represents the shear crack. In the laboratory test, we received the AE characteristics of basalt. Since the AE event generally corresponds to the microcrack, the AE counts reflect the information about microcracks indirectly in the rock under stress. (1) There are few or no AE events at the primary stage, which is mainly attributed to the friction of initial crack closure. (2) When the stress reached about 60% of peak stress, significant AE activity was observed.
due to the steady growth of the crack. (3) The AE activity increased rapidly near the peak stress, indicating the unstable growth of the crack. In the corresponding numerical simulation, there are no cracks in the initial pressure stage. With the increment of axial pressure, the weak bonds start to break. The formed cracks distribute randomly in the sample, leading to stress concentration in adjacent units. Meanwhile, the microcracks begin to nucleate and propagate, see in figure 8b.
When the loading stress reaches a certain level, the stress concentration of the particles becomes more obvious, resulting in a sharp increase of crack numbers. Both the AE activity in laboratory test and the crack propagation in numerical simulation can reveal the failure mode in basalt, see in figure 9. The cracks under low stress level have little influence on stress redistribution of the sample. With the increase in number of bonds broken, the stress redistribution and stress concentration phenomenon will be more obvious, leading in turn to the acceleration of crack propagation. Therefore, local shear fracture becomes obvious after passing the peak stress, developing into a damage zone as the final stage of specimen failure. It is the propagation, nucleation and penetration of microcracks that eventually lead to the compressive failure of basalt. As can be seen in figure 8, the crack before peak strength was mainly a tensile crack, and there was almost no shear crack. When reaching the peak strength, both tensile and shear crack increased rapidly. The total number of cracks is 1812, of which the number of tensile cracks is 1696 and the shear crack number is 116. The tensile crack is always dominant during the whole failure process. The numerical results presented here indicated that it is more likely a tensile rather than a shear process that caused the formation of the macroscopic fracture plane of basalt.

4.2. Energy conversion

Energy conversion is the essential characteristic of rock destruction. Rock deformation and failure is a process from local energy dissipation to local failure and eventually to global catastrophic failure, involving energy dissipation and energy release. Energy dissipation of rock is mainly composed of friction in microcrack closure, nucleation and penetration of microcracks and relative dislocation of a fracture surface under compression.

The damage process of basalt can be monitored by AE technology. AE activity is attributed to the rapid release of stored elastic energy due to the generation of new cracks or the growth of existing cracks in rock. Energy conversion at each stress level and the curve of the cumulative AE energy is showed in figure 10. The brittle failure of basalt has experienced absorption, accumulation, dissipation and release of energy. Before crack initiation (point A), there is no strain energy released during the closure of existing cracks. With the increment of loading, the strain energy stored in rock increases, leading to the initiation and stable expansion of the crack. When the strain energy accumulates in rock reaching a critical value (point B), the cumulative AE energy begins to release rapidly and the cracks extend unstably, eventually leading to the failure of rock.

Although the AE data contain microscopic fracture information, it could not reveal the damage mechanism well. We can only speculate on the internal energy conversion process and damage mechanism from this AE information. PFC can realize real-time recording of a system’s energy evolution process through the built-in FISH language. During the simulation, various energies are tracked to investigate the law of energy evolution during crack propagation, and to further understand rock fracture mechanics. The model provides three energy partitions: strain energy, stored in the
linear springs; bond strain energy, stored in the parallel-bond springs and slip energy, defined as the total energy dissipated by frictional slip. In the present model, once a bond is broken the energy will be released.

During the simulation, we also monitored the total input energy of a system, called boundary energy. The variation curves of energy are shown in figure 11. At the initial stage, the energy input from outside is mainly converted to strain energy, which is stored in two ways, in linear springs and parallel-bond springs. Because of the absence of a defect compaction stage in numerical simulation, almost all the energy is used for elastic deformation of the grain framework. During this period, the strain and bond strain energy showed a nonlinear and parabolic increase. In the meantime, the slip energy remained equal to zero until the bond broke. In the second stage, as the input energy increased, the strain energy stored in linear springs and parallel-bond springs continued to increase. In this stage, the bonds between particles started to break, resulting in the release of the strain energy stored in bonds. At this point, the slip energy started to appear because it is the sum of the frictional actions of cracks. The slip energy was activated only after microcracks formed and it increased with crack propagation. In the last stage, as shown in figure 11, elastic strain energy and the parallel-bond strain energy continued to grow when the energy exceeded the limit most springs find acceptable, most of the bonds broke and the strain energy stored in the springs was released quickly. At this time, the slip energy showed a rapid increase, because the bearing capacity of the sample mainly depended on the sliding friction between particles.

The total energy input into the system consists of two parts: \( E_s \), the elastic strain energy stored in the rock and \( E_p \), the dissipative energy for rock damage and plastic deformation. The dissipative energy can be defined as follows:

\[
E_p = U - E_s
\]  

5. Conclusion

In this paper, a PFC2D model is suggested to investigate the microscopic mechanism of basalt failure under uniaxial compression. Based on the AE experiment and numerical simulation data of basalt, crack evolution and energy conversion in specimen are studied in detail. The following conclusions can be made:

![Figure 10. AE accumulated energy.](https://example.com)
(1) Under uniaxial compression, the deformation of basalt was mainly elastic deformation without an obvious yield process before the peak stress.

(2) The types and number of microcracks were calculated during numerical simulation. The cracking pattern in the basalt model was close to that observed in the laboratory test; namely, that cracks were predominantly tensile and oriented parallel to the loading direction. The AE experiment and numerical simulation revealed that different deformation stages of basalt corresponded to different characteristics of microcrack propagation.

(3) The various energies during the failure process were monitored. The intermittent breakage of bonds in the numerical simulation were similar to sources of AEs in real experiments. In the stage of rock compaction and elastic deformation, the AE energy was at very low level. Accordingly, the input energy was all converted to strain energy stored in the bonds of numerical.

Figure 11. Energy conversion in a numerical simulation.
simulations. When the sample reached its peak strength, a large amount of AE energy was monitored in experiments and the strain stored in bonds declined rapidly due to bond breakage.

The dislocation and breakage of bonds gave rise to the crack propagation and penetration, eventually leading to the reduction of macroscopic mechanical parameters and the deterioration of mechanical properties. This helps give more confidence in the behavior of the model, so that it can be used to investigate the micromechanics that combine to produce complex macroscopic behaviors and as an engineering tool to predict these macroscopic behaviors.

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