Modeling Grain Size Heterogeneity Effects on Mechanical Behavior of Crystalline Rocks Under Compressive Loading

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Abstract

Strength and deformation behavior of intact rocks is influenced by a large number of factors, notably mineralogical content. If the constituent minerals are strong, the overall rock strength will be high, and vice versa. The prediction of rock properties of those composed of different types and amounts of minerals will be difficult. This paper presents a numerical approach to study the influence of material heterogeneity associated with the variation of grain size distribution and shape on the strength and deformation behavior of a felsic crystalline rock. By taking advantage of a grain-based modeling approach in two-dimensional Particle Flow Code, a heterogeneity index is defined and explicitly incorporated into the numerical models quantitatively. The numerical results reveal that the peak strength increases as the numerical model gradually changes the character of the rock from heterogeneous to homogeneous. The number of grain boundary tensile cracks gradually decreases and the number of intra-grain cracks increases at the moment of failure. The orientation of grain boundary micro-cracks is mainly controlled by the geometry of assembled grain structure of the numerical model, while the orientation of intra-grain micro-cracks is to a large degree influenced by the confinement. In addition, the development of intra-grain cracks (both tensile and shear) is much more favored in quartz than in other minerals. The findings of this study provide insights to the interpretation of rock properties, particularly those which are strongly influenced by the heterogeneous mineralogical composition.

1 Introduction

Rock is typically heterogeneous composed of different types of minerals and inherent microstructures. Laboratory test results indicate that the strength and deformation responses and the associated micro-cracking behavior of rocks are to a large extent affected by the internal microstructures-induced heterogeneity (Brace et al. 1966; Eberhardt et al. 1998; Fredrich et al. 1990; Martin and Chandler 1994). Therefore, the mineral assembly induced rock material heterogeneity is an important factor that needs to be considered when studying the micro-cracking behavior of rocks.

In general, two approaches are available for incorporating material heterogeneity into numerical models when investigating the cracking processes of rocks. In the first approach, which is known as the implicit approach, the material heterogeneity is implicitly incorporated via a stochastic distribution of rock properties, such as the Weibull distribution based models and the Lattice model (Tang et al. 2000; Blair and Cook 1998; Schlangen and Garboczi 1997). These implicit modeling methods have demonstrated that heterogeneity has a great influence on the mechanical behavior of rocks. However, the choice of input properties is to some extent subjective and highly dependent on the parameters in the statistical distribution. In the second approach, which is known as the explicit approach, the heterogeneity is explicitly described in the numerical specimen model to be simulated, such as grain-based models implemented into Universal Distinct Element Code (UDEC) (Lan et al. 2010) or two-dimensional Particle Flow Code (PFC2D) (Potyondy 2010), combined finite-discrete element

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method (Mahabadi et al. 2014), and explicit finite element method (Manouchehrian and Cai 2016).

In a recent study by Peng et al. (2018), the grain-based modeling approach in PFC2D was demonstrated to be promising for studying the micro-cracking behavior of crystalline granitic rocks. This model is used in this study to further investigate the influence of rock material heterogeneity on the strength and micro-cracking behavior of a crystalline rock. The heterogeneity induced by variation of grain size distribution and shape is explicitly incorporated into the numerical specimens quantitatively by a "heterogeneity index". The rock strength and deformation behavior and the associated micro-cracking process of numerical models with different heterogeneity indices are then examined and discussed.

2 Methodology

2.1 Grain-Based Modeling Approach in PFC2D

The grain-based modeling approach in PFC2D which was proposed by Potyondy (2010) is used in this study to investigate the material heterogeneity effect on rock strength and micro-cracking behavior. The micro-properties in a real rock, such as grain size distribution and mineralogical composition, can be reflected in the grain-based model. The PFC2D grain-based modeling approach generates polygonal grain structure which is representative of the crystalline rocks. Two contact models are used in the grain-based model. The discs inside the grains are bonded by parallel bonds and the discs along the grain interfaces are assigned with the smooth-joint contacts.

The details of generating a grain-based model in PFC2D are not presented here. Interested readers can refer to Potyondy (2010) or Peng et al. (2018). The PFC2D grain-based model can not only simulate the micro-crack initiation and interaction at the grain boundary, but also capture the micro-cracking behavior inside the grains which is associated with intra-granular micro-cracking. This approach has been demonstrated to be capable of simulating the failure behavior and micro-cracking process of crystalline rocks (Bahrani et al. 2014; Bewick et al. 2014; Hofmann et al. 2015).

2.2 Numerical Model Setup

In this study, the numerical model comprises four minerals (quartz, K-feldspar, plagioclase, and biotite) which is the same as that simulated by Peng et al. (2018). Grain sizes of different minerals are generally different. The average grain size R_a of a numerical model is expressed as

$$R_a = \sum_{i=1}^{m} \omega_i r_i \tag{1}$$

where ω_i and r_i are the volume fraction and mean grain size of different constituent minerals, respectively, and m is the number of associated mineral types.

In order to study the influence of material heterogeneity, which is induced by the variation of grain size distribution, on rock strength and micro-cracking behavior, a dimensionless heterogeneity index H is defined as

$$H = \sqrt{\sum_{i=1}^{m} \left(\frac{r_i}{R_a} - 1 \right)^2} \tag{2}$$

By changing the grain size of different minerals that constitute a rock, numerical models with different heterogeneity indices can be generated. According to the definition of the heterogeneity index, a larger heterogeneity index represents a more heterogeneous model. Table 1 shows the mean grain sizes of minerals r_i and the heterogeneity indices H for the six different numerical models investigated in this study. The average grain sizes R_a of the numerical models are basically the same, while the heterogeneity indices range from 0 to 1.12.

In a former study by Peng et al. (2018), the micro-cracking behavior of Singapore Bukit Timah granite (BTG) was simulated using the PFC2D grain-based model. The studied BTG was composed of approximately 22.3% K-feldspar, 30.4% quartz, 36.3% plagioclase, and 10.7% biotite. It was found from previous laboratory test results that the mineralogical composition had a great influence on the mechanical properties of rocks (Güneş Yılmaz et al. 2011; Sajid et al. 2016). To avoid the influence of mineralogical composition on the simulation results in this paper, we assign the content of each mineral with equal value, i.e., 25.0%, at the early development of the model. However, due to truncation by the specimen boundary, some grains along the periphery are smaller than the designated grain size, leading to the fact that the content of each mineral is not exactly 25.0%.

The dimensions of the present generated numerical specimen models are 50 mm in length and 25 mm in width, which are the same as those simulated by Peng et al. (2018). They are smaller than those experimentally tested (100 mm long and 50 mm wide). According to Potyondy and Cundall (2004), if the particle size is relatively small as compared to the size of the model, the scale effect is not significant for modeling rocks in compressive loading conditions. Reducing the size of the numerical model will thus not significantly affect the simulation results and conclusions, but can improve the computing efficiency. The numerically-generated models of different heterogeneity indices (H) are presented in Fig. 1.

Table 1 Parameters for the generated numerical grain-based models

Specimen no.	R_a (mm)	H	Mean grain size of minerals r_i (mm)			
			K-feldspar	Quartz	Plagioclase	Biotite
HE1	2.1	1.12	3.0	1.5	3.5	0.5
HE2	1.9	1.02	2.5	1.5	3.0	0.5
HE3	2.0	0.79	2.5	1.5	3.0	1.0
HE4	1.9	0.69	2.5	1.5	2.5	1.0
HE5	2.0	0.35	2.0	2.0	2.5	1.5
HE6	2.0	0	2.0	2.0	2.0	2.0

| $H = 1.12$ | $H = 1.02$ | $H = 0.79$ | $H = 0.69$ | $H = 0.35$ | $H = 0$ |
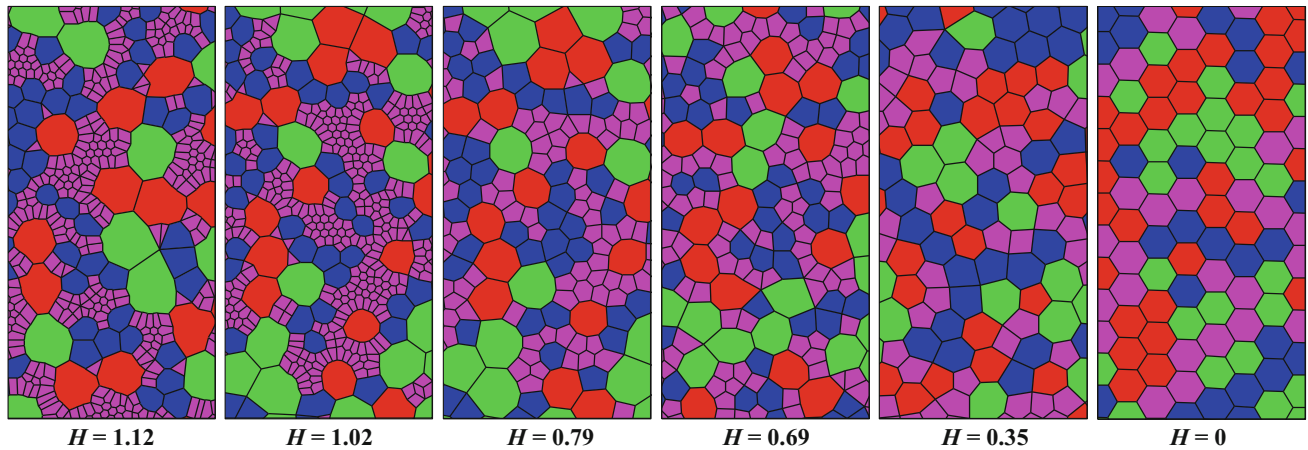
Fig. 1 Numerical models with different heterogeneity indices. The colors indicate different mineral types (red = K-feldspar, blue = quartz, green = plagioclase, magenta = biotite). The specimen dimensions are 50 mm in length and 25 mm in width

Note that when $H = 0$, the model is homogeneous, consisting of uniformly packed regular hexagons.

The micro-parameters of BTG were calibrated by Peng et al. (2018) to match a number of macro-properties of the BTG tested in the laboratory, including direct tensile strength (σ_{dt}), UCS, Young's modulus (E), and compressive strengths under various confining pressures. The results revealed that the errors between the laboratory properties and the simulated values using grain-based model were within ±6%. The well-calibrated micro-parameters are used in this study to investigate the strength and micro-cracking behavior of models processing different numbers of heterogeneity indices.

Fig. 2 Strength evolutions of numerical models with the heterogeneity index

3 Simulation Results

3.1 Rock Strength Behavior

The strength variations of the numerical models with the heterogeneity indices are illustrated in Fig. 2. The material heterogeneity also has a g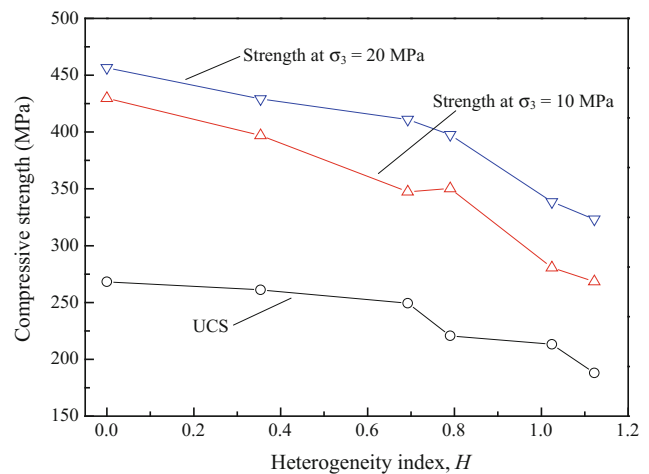reat effect on the rock strength under compressive loadings. The compressive strength gradually decreases as H increases from 0 to 1.12, i.e., the more heterogeneous the numerical model is, the lower the compressive strengths will be.

3.2 Number of Micro-cracks

Figure 3a–c presents the number of four different types of micro-cracks at the end of the loading process of the numerical models under different loading conditions. The grain boundary tensile cracks are found to dominate among the generated micro-crack types, indicating that the failure mechanism is attributed mainly to tensile cracking under low confining pressures. The number of grain boundary tensile cracks generally decreases with the decrease of H from 1.12 to 0 under compressive compression. However, there is no obvious trend for the development of other types of micro-cracks.

The total number of generated micro-cracks is also computed and summarized (Fig. 3d). The results reveal that when the heterogeneity index is large (i.e., HE1 and HE2), the total number of micro-cracks increases with the increase of confining pressure. However, as the heterogeneity index becomes lower, the total numbers of generated micro-cracks are very similar for different confining pressures.

3.3 Orientation of Micro-cracks

Figure 4 illustrates the orientation distribution of generated "**grain boundary micro-cracks**" for numerical models with different heterogeneity indices under uniaxial compression. The results reveal that the orientation of grain boundary micro-cracks is significantly affected by the grain size distribution induced heterogeneity, which is associated with the geometry of assembled grain structure of the numerical model. The following phenomena are observed:

- When the heterogeneity index is large, the grain boundary micro-cracks are mainly generated approximately parallel to the vertical direction.
- As the heterogeneity index decreases, although most of the generated grain boundary micro-cracks are oriented in the vertical direction, more and more micro-cracks are found to be inclined at about 60°–75° and 105°–120°.
- When the numerical model is homogeneous ($H = 0$), most of the grain boundary micro-cracks are generated at
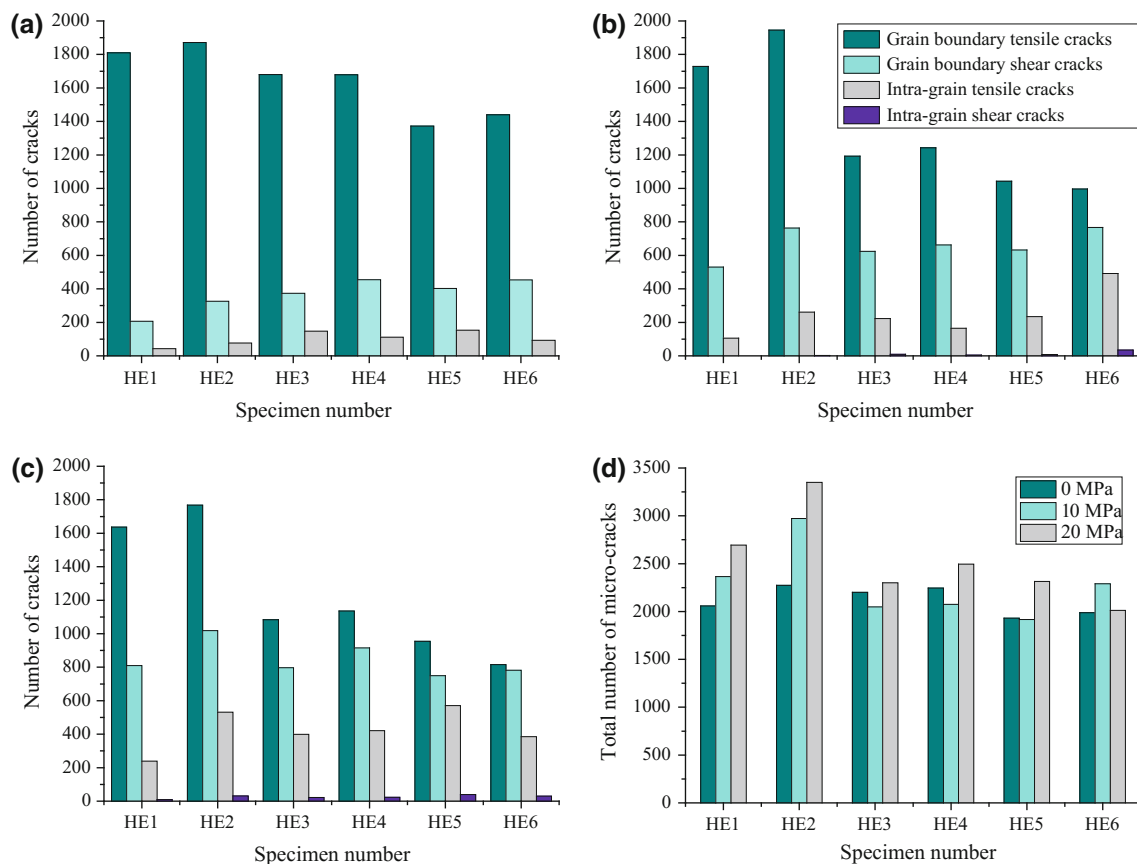

Fig. 3 Number of different types of generated micro-cracks for different numerical models under confining pressure of **a** 0 MPa—uniaxial compression. **b** 10 MPa. **c** 20 MPa. **d** Total number of generated micro-cracks for different numerical models
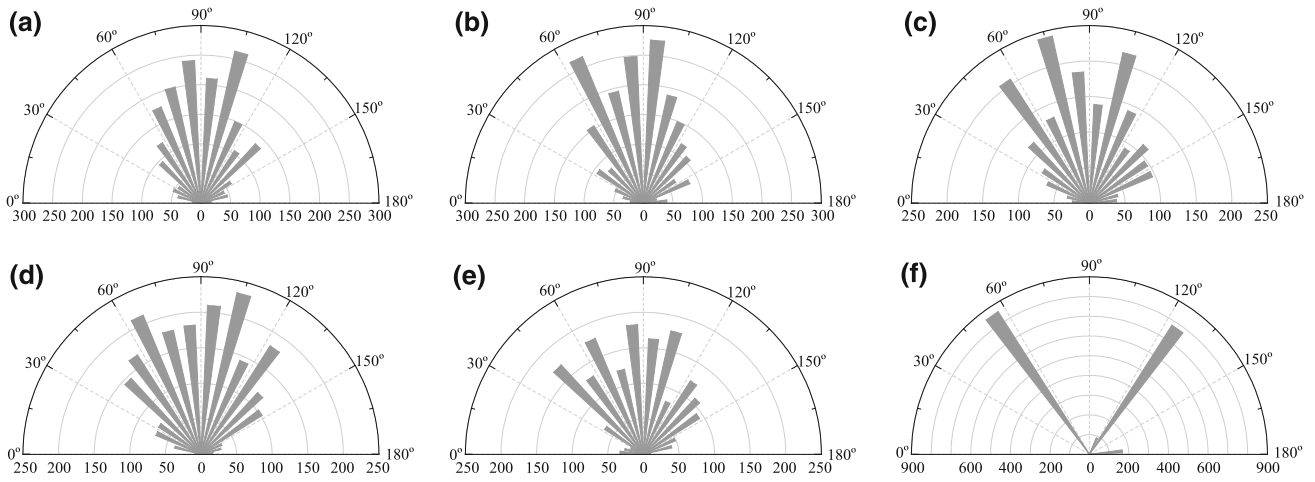
Fig. 4 Orientation distribution of the generated grain boundary micro-cracks in the numerical models with different heterogeneity indices under uniaxial compression. **a** HE1: $H = 1.12$. **b** HE2: $H = 1.02$. **c** HE3: $H = 0.79$. **d** HE4: $H = 0.69$. **e** HE5: $H = 0.35$. **f** HE6: $H = 0$

about 60° and 120°. The phenomenon is mainly due to the general association of the grain boundary micro-cracks and the grain interfaces in the generated numerical models. As shown in Fig. 1, as the numerical model becomes more homogeneous, more grain interfaces tend to be inclined at about 60°–75° and 105°–120°.

The orientation distribution of generated "**intra-grain micro-cracks**" of different numerical models under uniaxial compression are presented in Fig. 5. The heterogeneity does not have a pronounced influence on the orientation of intra-grain micro-cracks, as compared with the results of grain boundary micro-cracks. Most of the generated

intra-grain micro-cracks incline approximately parallel or slightly inclined to the vertical loading direction.

Figure 6 presents the variations of orientation of "**grain boundary micro-cracks**" and "**intra-grain micro-cracks**" with the confining pressure for the numerical model of H = 0.69. The rose diagrams reveal that the orientation of grain boundary micro-cracks are generally the same under different confining pressures, indicating that the influence of confinement is not significant. On the other hand, the orientation of intra-grain micro-cracks seems to be greatly affected. When the numerical model is loaded under uniaxial compression, most of the intra-grain micro-cracks are generated along the vertical direction. With increase of the
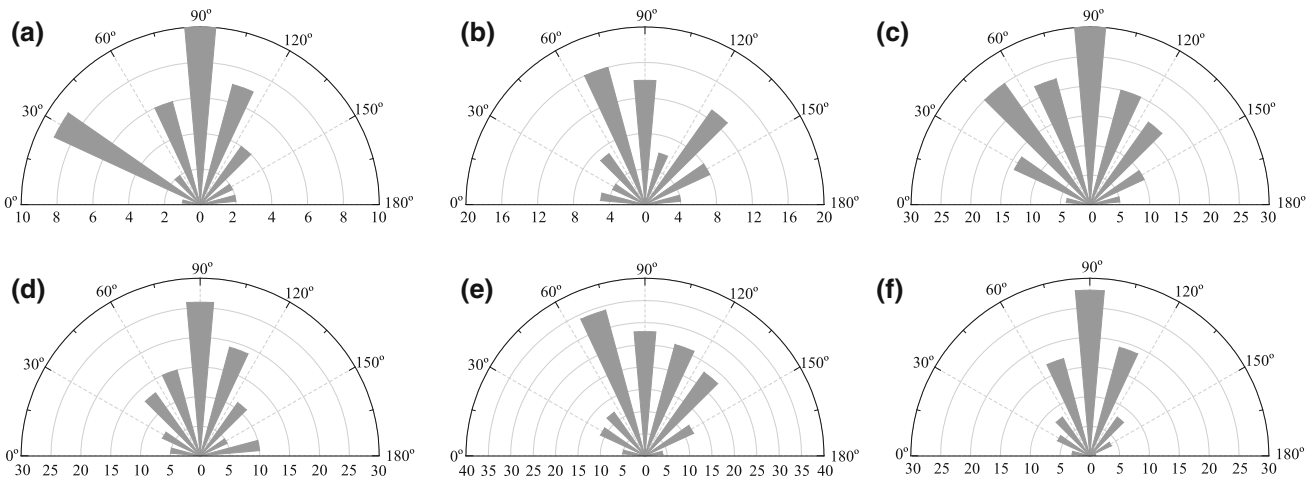

Fig. 5 Orientation distribution of the generated intra-grain micro-cracks in the numerical models with different heterogeneity indices under uniaxial compression. **a** HE1: $H = 1.12$. **b** HE2: $H = 1.02$. **c** HE3: $H = 0.79$. **d** HE4: $H = 0.69$. **e** HE5: $H = 0.35$. **f** HE6: $H = 0$
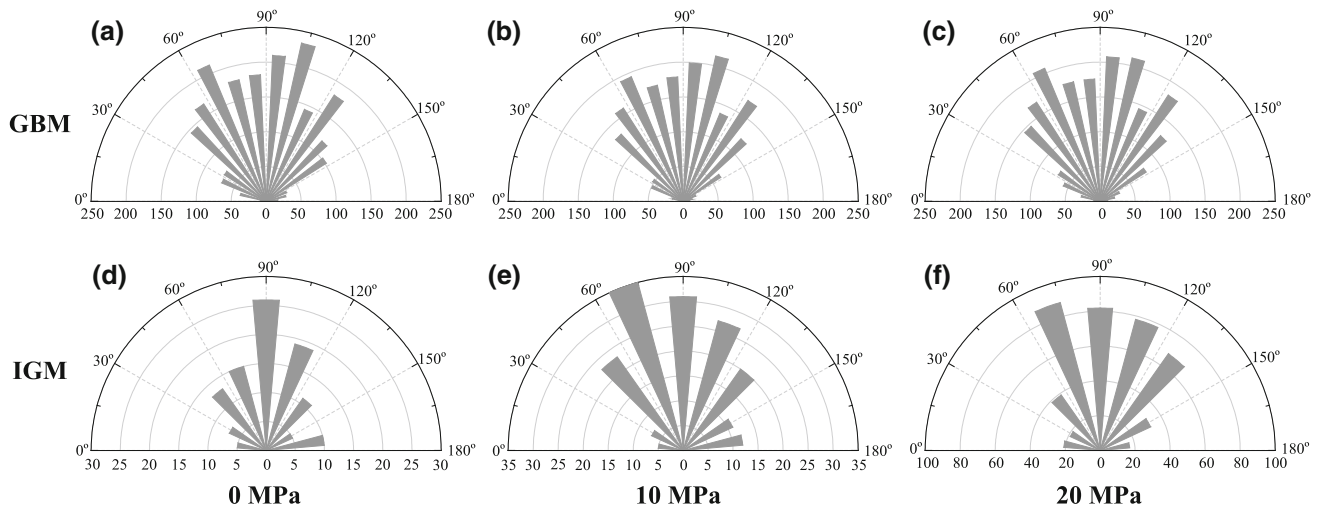
Fig. 6 Orientation distribution of two types of micro-cracks in the numerical model HE4 ($H = 0.69$) under various confining pressures. Grain boundary micro-cracks under confining pressure of **a** 0 MPa, **b** 10 MPa, **c** 20 MPa; Intra-grain micro-cracks under confining pressure of **d** 0 MPa, **e** 10 MPa, **f** 20 MPa. (GBM: grain boundary micro-crack; IGM: intra-grain micro-crack)

confining pressure, more intra-grain micro-cracks are found to incline at about 30° along the loading direction.

3.4 Pattern of Micro-cracks

The spatial distributions of different types of micro-cracks for numerical models with different heterogeneity indices under uniaxial compression are presented in Fig. 7. When the heterogeneity index is relatively high, the generated micro-cracks are generally uniformly distributed in the model, with the orientation of micro-cracks varying in a relatively large range. As the numerical model becomes more homogeneous, the interaction of generated micro-cracks tends to form more macroscopic fractures which are oriented approximately in the vertical direction. Because the homogeneous numerical model ($H = 0$) is

uniformly assembled with regular hexagons, when the numerical model is loaded, the micro-cracks are generally generated along the sub-vertical grain interfaces, which will eventually form vertical macroscopic fractures. The lateral dilation in this condition is much larger than those with large heterogeneity indices.

The distributions of different types of micro-cracks for different heterogeneity indices under the confining pressure of 20 MPa are shown in Fig. 8. As compared with the results under uniaxial compression, more intra-grain cracks develop in the model due to the higher applied confining pressure. When the crack density is sufficiently high, the interaction and coalescence of grain boundary micro-cracks and intra-grain micro-cracks lead to the formation of macroscopic shear bands. The results are in good agreement with microscopic observation of the Westerly granite by Moore and Lockner (1995). When the heterogeneity index is large, the
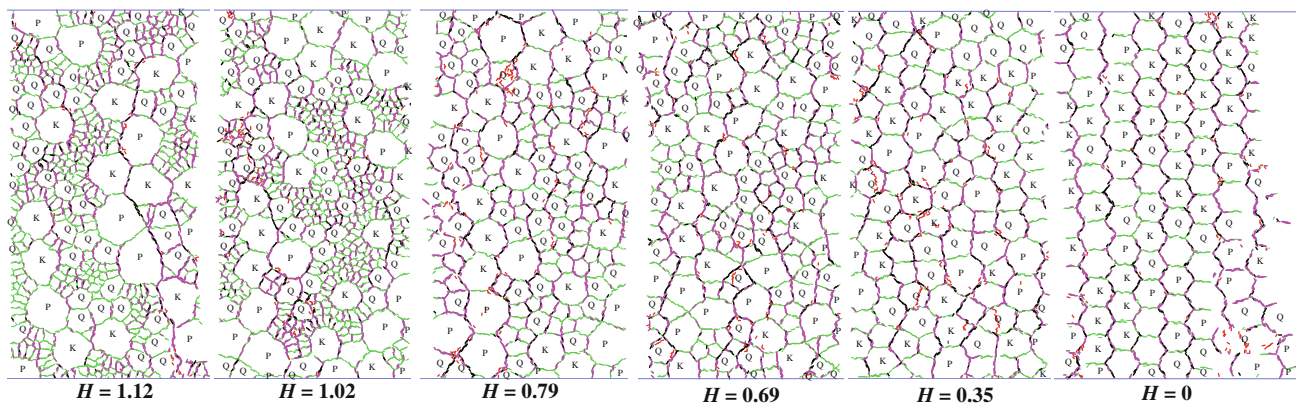

Fig. 7 Micro-cracking behavior of the numerical models with different heterogeneity indices under uniaxial compression. The different minerals are identified (Q: quartz, K: K-feldspar, P: plagioclase, and biotite is not labelled). Green segments represent grain boundaries, magenta and black segments represent grain boundary tensile and shear cracks, respectively, and red segments represent intra-grain tensile cracks
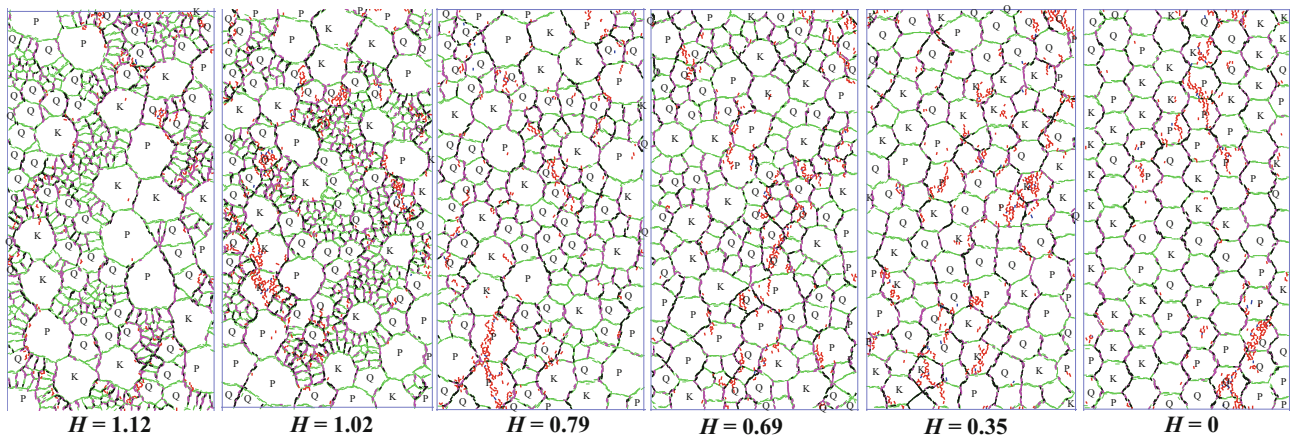
| $H = 1.12$ | $H = 1.02$ | $H = 0.79$ | $H = 0.69$ | $H = 0.35$ | $H = 0$ |

Fig. 8 Micro-cracking behavior of the numerical models with different heterogeneity indices under the confining pressure of 20 MPa. The different minerals are identified (Q: quartz, K: K-feldspar, P: plagioclase, and biotite is not labelled). Green segments represent grain boundaries, magenta and black segments represent grain boundary tensile and shear cracks, respectively, and red and blue segments represent intra-grain tensile and shear cracks, respectively

generated micro-cracks are found to be relatively uniform. As the numerical model becomes more homogeneous, more intra-grain cracks develop in the model and the induced macroscopic shear band is more prominent than the results of numerical models with much higher heterogeneity indices.

The simulation results also show that most of the intra-grain cracks (both tensile and shear) generally develop in quartz (except the numerical models with heterogeneity indices equal to 0.35 and 0.79 under the confining pressure of 20 MPa). This is mainly due to the fact that the particle-particle contact modulus, and parallel bond modulus and strength in the quartz mineral are assigned with the highest value as compared with the values of other minerals (Peng et al. 2018). Many researchers investigated the micro-cracking behavior of crystalline rocks and found that the intra-grain cracks occurred mostly in quartz grains (Tullis and Yund 1977). These observations are in good agreement with the simulation results in this study.

4 Conclusions

This paper numerically investigates the influence of grain size heterogeneity on the micro-cracking process and strength of a crystalline rock. The simulation results reveal that the peak strength generally increases as the numerical model gradually progresses from heterogeneous to homogeneous. The micro-cracking behavior is also found to be greatly affected by material heterogeneity. As the numerical model becomes more homogeneous, the number of generated grain boundary tensile cracks gradually decreases and the number of intra-grain cracks (both tensile and shear) increases. The orientation of grain boundary micro-cracks is mainly controlled by the geometry of assembled grain

structure of the numerical specimen model, while the orientation of intra-grain micro-cracks is to a large degree influenced by the confinement. The results also reveal that the development of intra-grain cracks (both tensile and shear) is much more favored in quartz than in the other minerals, which is generally in good agreement with the previous laboratory test results by other researchers.

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