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Grain-Based Modeling Of The Macro-Mechanical Behavior Of Crystalline Rock Considering The Heterogeneity Of Grain Boundary Contacts

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Abstract – Grain-Based Model (GBM) based on the Discrete Element Method (DEM) has been widely used to simulate the rock specimen under load realistically. A common problem in the current implementation of GBM is that only a single bond parameter is used on the grain boundaries. However, there are several minerals present in the rock specimens. For this purpose, this study focuses on accurately simulating the rock specimen based on the GBM model by considering various grain boundary contacts between different minerals. A GBM was proposed and incorporated into the Particle Flow Code (PFC), which can capture the intergranular textures of rock. The model is applied to reproduce the laboratory response of Lac du Bonnet granite. An iterative calibration approach is developed to match the unconfined compressive (UCS) of the models to those of the laboratory results. The transition in the failure mode, stress-strain response, and the evolution of inter and intra-grain micro-cracks were systematically examined and compared with those derived from the traditional model with a single bond parameter for grain boundary. The results show that the inter cracks are more dispersed in the specimen in the new model, especially at the pre-peak stage. At the post-peak stage, inter-grain tensile and shear cracks still dominate the microcrack distributions in the traditional model; in contrast, the intra-grain cracks dominate the microcrack distributions in the new model. The order in which the micro-cracks appear significantly differs between traditional approaches and the new model.

***Keywords*:** Grain-Based Model**;** Grain boundary contacts; DEM; crystalline rock

1. Introduction

Rock is a heterogeneous material because it is composed of various materials (i.e., mineral and cements) and microstructural defects (i.e., microcracks) (Liu et al., 2018). Rock specimens of the same rock type may exhibit different crack propagation behavior due to grain-scale heterogeneity and hence different strengths (Martin and Chandler 1994). Generally, grain-scale heterogeneity includes heterogeneity of mineral content, shape, size, and spatial distribution, and pre-existing defects in the form of voids, microcracks, weak grain boundaries, and cleavages. Over the past several decades, many scholars have used GBM within DEM method to investigate the effect of rock heterogeneity on the strength and deformation of the specimen (Zhao et al., 2021). It is widely accepted that heterogeneity is vital in generating localized tensile stresses resulting in crack propagation

Although the effect of grain-scale heterogeneity on the deformation behavior and strength characteristics of rock material has been widely studied, much less attention has been dedicated to the heterogeneous strength of grain boundaries. GBM-based DEM method has shown significant advantages in reproducing grain-scale heterogeneity in the rock. A common problem in the current implementation of GBM is that the grain boundaries are simulated with only a single contact parameter. Several minerals are present in the rock specimens, and the property of grain boundaries between any two minerals should be different.

This study aims to accurately simulate the rock specimen based on the GBM model by considering various grain boundary contacts between different minerals. The GBM numerical modeling using the PFC (Particle Flow Code) developed by Itasca (2021) is used to capture the grain-scale heterogeneity in the rock and to reproduce the macro-properties of the Lac du Bonnet granite. PFC models are fabricated to assign various bond parameters to grain boundary contacts. By performing numerical tests on specimens with heterogeneous grain boundary contacts, rocks' inter and intra-crack propagation, deformation response, and failure mode were numerically examined.

2. PFC-GBM model

For the GBM model in this study, two different contact models were used to mimic the bond effect of intragrain texture (mineral grains) and the grain boundary (minerals boundary), respectively. The discs in each polygonal mesh are bonded by the Flat-Joint Model (FJM) in PFC (Itasca, 2021) to form a mineral grain of crystalline rock. The FJM parameters within a grain vary with the type of minerals. They were calibrated to reproduce the macro-properties of each mineral. A weak linear parallel bonded model (LPBM) (Itasca, 2021) was used to model the contact of grain boundaries. To consider the heterogeneity of grain boundary contact in the GBM model, the parameters for the LPBM contact vary with every two types of minerals. Parameter calibration Calibration procedures for the GBM are similar to the methods recommended by Zhao et al. (2021). The detailed calibration process can be seen in Zhao et al. (2021). The contact parameters on the grain boundaries are assigned with the mean values of the two contacting minerals and multiplied by the attenuation coefficients. This way, the heterogeneity of grain boundary contact and the weaker bond property of the boundary can be achieved.

3. Modeling Lac du Bonnet (LdB) granite

3.1. Calibration of Unconfined Compressive Strength (UCS)

As shown in Fig. 1(a), LdB granite is a typical brittle rock. It comprises four main minerals: alkali feldspar (48%) (mineral_1), plagioclase (17%) (mineral_2), quartz (29%) (mineral_3), and biotite (6%) (mineral_4), with mean grain diameters of each mineral as 4, 4, 2, and 1 mm, respectively (Martin and Chandler 1994).

The dimensions of the GBM in PFC for UCS test are 100 mm (height) and 50 mm (width), which is consistent with the standard experimental size of the physical rock specimens. The grain diameters of the GBM are: alkali feldspar (4 mm), plagioclase (6 mm), quartz (3 mm), and biotite (2 mm). The grain's minimum and maximum particle sizes are set as 0.15 mm and 0.25 mm, respectively. The number of particles comprising the GBM specimen is 20,325. The GBM in PFC for the UCS test is shown in Fig. 1(b), (c). The calibrated grain and grain contact property parameters of LdB granite are given in Table. 1.

Table 1: Calibrated grain and grain contact property parameters of LdB granite

Microscale parameters for minerals	Plagioclase	Alkali feldspar	Quartz	Biotite
Effective density / ρ (kg/m^3)	2600	2500	2700	2850
Effective modulus / E_c (GPa)	53.37	70.18	73.76	100.29
Normal to shear stiffness ratio / k_c	1.5	1.5	1.5	1.5
Friction angle / φ_f (∘)	10	13	2	10
Bonded tensile strength / σ_t (MPa)	34.63	45.4	76.51	14.6
Bonded cohesion / c_b (MPa)	235.77	289.6	474.7	220.4
Number of elements in the radial direction / N_r	4	4	4	4
Microscale parameters of grain boundary				
Attenuation coefficient of modulus / α_E	Attenuation coefficient of normal to shear stiffness ratio / α_k	Attenuation coefficient of friction angle / α_φ	Attenuation coefficient of tensile strength / α_t	Attenuation coefficient of cohesion strength / α_c
2.0	6.0	1.0	0.5	0.15

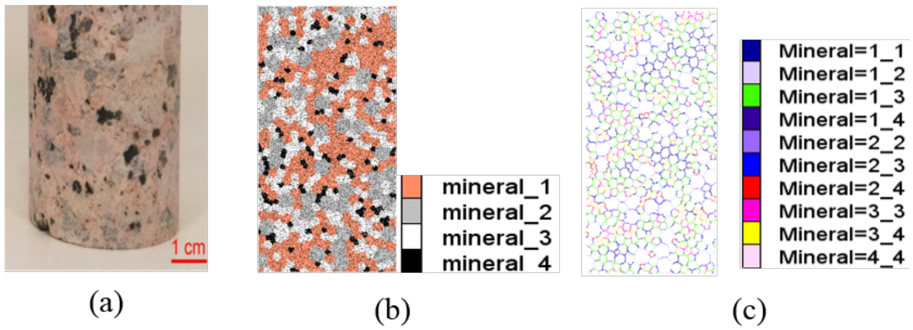

Fig. 1. (a) Granite (modified from Nicco et al. 2020); (b) LdB granite grain texture model in PFC (GBM); (c) Heterogeneity of grain boundary contact in PFC

The stress-strain curves for uniaxial compression and tensile tests are shown in Fig. 2. It is shown that the UCS, Young's modulus (E) and Poisson's ratio (v), volumetric strain (V_{strain}) are overall consistent with that LdB granite, which confirmed that the GBM with the calibrated grain and boundary contact property can be used to study the macro and micro behavior of LdB granite.

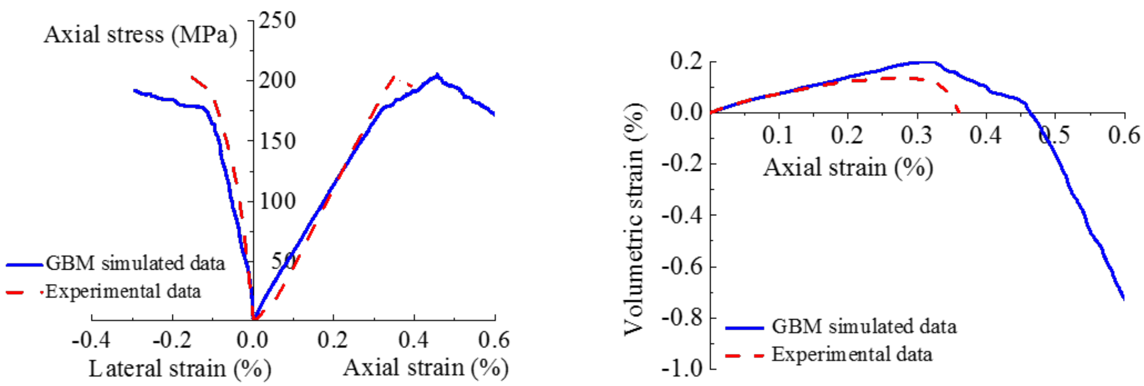

Fig. 2. Comparison between the experimental data reported by Martin and Chandler (1994) and the results of GBM

3.2. Microcrack propagation

Fig. 3 shows the microcrack distributions in the specimen at different stages under the uniaxial compressive test. The results derived from a similar GBM model but with only a single contact parameter for grain boundary (traditional model) were also presented for a direct comparison. It can be seen that most microcracks propagate and extend along the axial direction, which is parallel to the maximum compressive stress. This result agrees with the observations in previous studies (Martin and Chandler, 1994;). In terms of the microcrack distribution, it is shown that the micro-cracks begin to propagate along the grain boundary in the form of tensile cracks. With the increment of compressive load, tensile microcracks appear in the mineral grains (intra-grain tensile cracks) and followed by the shear microcracks appear at the grain boundary (inter-grain shear cracks) as well as in the mineral grains (intra-grain shear cracks). A comparison with the results of the traditional model shows that the inter cracks are more dispersed in the specimen in the new model, especially at the pre-peak stage. At the post-peak stage, inter-grain tensile and shear cracks still dominate the microcrack distributions in the traditional model; in contrast, the intra-grain cracks dominate the microcrack distributions in the new model. Fig. 3 presents the increase of crack number as a function of axial strain. The results of the traditional model are also presented (Fig. 3 (a)) for comparison. As expected, for both models, the tensile inter-grain cracks appeared first. With the increasing compressive load, the traditional model detected the appearance of shear inter-grain cracks followed by intra-grain cracks. In contrast, the intra-grain tensile cracks were observed, followed by intra-grain and inter-grain shear cracks in the new model.

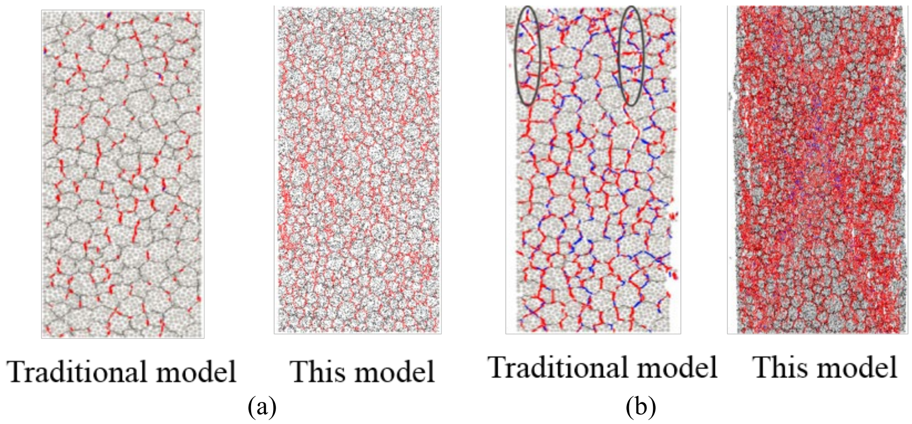

Fig. 3. Microcrack distributions in specimens during the uniaxial compressive test: (a) Pre-peak stage at a strain level of 0.1%. (b) Post-peak stage at which the axial stress is 80% of the peak strength. Black, red, and blue lines indicate grain boundary, tensile, and shear micro-cracks, respectively. The results of the traditional model are adapted from Liu et al. (2018)

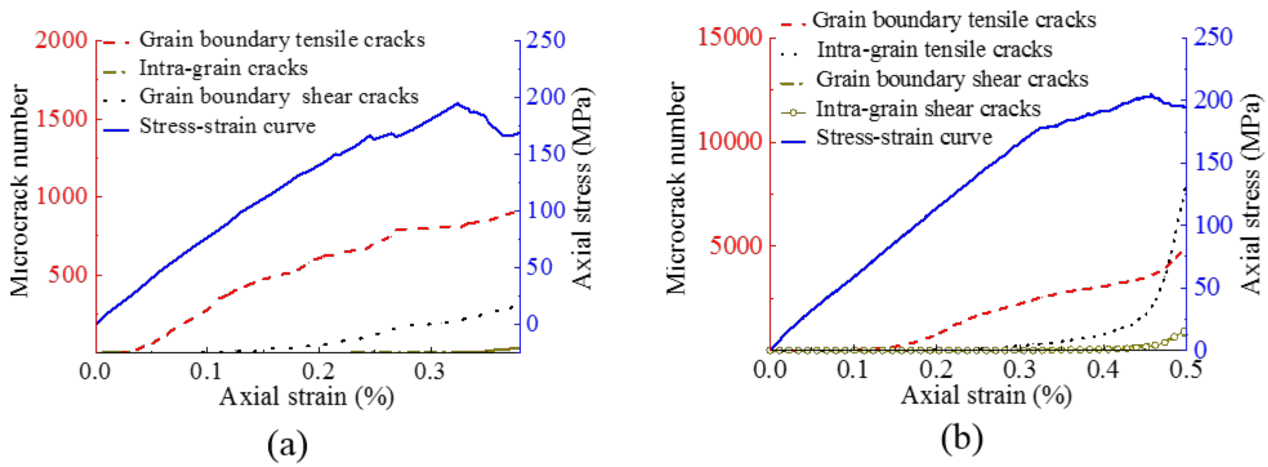

Fig. 4. Crack number–axial strain and stress-strain curves for specimens: (a) Traditional model with a single bond parameter for grain boundary (adapted from Liu et al., 2018); (b) New model with the various bond parameters for grain boundary. Note that the intra-grain cracks shown in the figure include tensile and shear cracks.

4. Conclusion

This research quantitatively studies the effect of the heterogeneous strength of grain boundaries on the mechanical properties and microcracking behavior of brittle rocks. A GBM model is applied to reproduce the UCS response of Lac du Bonnet granite. The transition in the failure mode, stress-strain response, and the evolution of inter-and intra-grain micro-cracks were systematically examined and compared with those derived from the traditional model with a single bond parameter for grain boundary. The following conclusions are summarized:

(1) During the unconfined compressive test, the inter-grain tensile cracks appeared firstly for both traditional and new models. The inter cracks are more dispersed in the specimen in the new model, especially at the pre-peak stage. At the post-peak stage, inter-grain tensile and shear cracks still dominate the microcrack distributions in the traditional model; in contrast, the intra-grain cracks dominate the microcrack distributions in the new model.

(2) The order in which the micro-cracks appear is significantly different between the traditional and new models. With the increasing compressive load, the order in which the micro-cracks appear in the traditional model is: inter-grain tensile cracks → Inter-grain shear cracks → intra-grain cracks. For the new model, the order is: inter-grain tensile cracks → intra-grain tensile cracks → intra-grain shear cracks →inter-grain shear cracks.

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