Understanding the Microscopic Mechanisms of the bi-modular behavior of rock

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ABSTRACT: Rocks when tested in both tension and compression show bi-modularity. Although the effect of all the factors contributing to the bi-modularity behavior is not fully understood, one of the main contributing factors is considered to be the presence of the micro-structure separating/joining the mineral grains. In this study, the effects of grain micro-structure on the modulus ratio are examined using the discrete element tool PFC2D for LdB granite and yellow sandstone. Extensive calibration was carried out to find out the intergranular micro properties of the mineral grains which produce the macroscopic response of the rocks. The role of inter-granular bond strength, initial micro-fractures present, and inter-granular bond stiffness were investigated. It was found that initial micro-fractures present in a rock sample is the main reason for producing the bi-modularity in rock and by considering it, crack initiation stress observed in the laboratory can be captured (~ 40% of UCS).

Keywords: Rock bi-modularity, micromechanical grain properties, PFC, crack initiation stress.

1 BACKGROUND

Natural rocks and man-made granular and fibrous composites display bi-modularity when subjected to compressive and tensile stresses. In rocks, the tensile Young's modulus is typically less than the compressive Young's modulus while for the fibrous composite materials like carbon, the tensile Young's modulus can be 2-5 times the compressive Young's modulus. The bi-modularity of rock is generally ignored for the numerical analysis and design of rock structures. To obtain the compressive Young's modulus (Ec) and Poisson's ratio of a rock, the ISRM Suggested Method for obtaining the deformability of rock materials in uniaxial compression (Bieniawski & Bernede, 1979) is used. While the ISRM suggested methods for determining the tensile strength of rock materials (ISRM 1978) is used to obtain Young's modulus (Et) and Poisson's ratio in tension. Also, the indirect three-point bending test and/or the Brazilian test have been used by Fairhurst, 1961; Ye et al., 2009; and Patel and Martin, 2018 to obtain the compressive and tensile Young's modulus and Poisson's ratio in the literature. The mean and standard deviation of the ratio between Et and Ec is shown in Figure 1.

As can be observed from Figure 1, the Et is always less than 1.0 (the mean varies from 0.27 to 0.72). This is true irrespective of the grain size of the rocks. However, for the fine-grain material, the ratio is close to one.

The reason for the bi-modularity of rocks is unknown. In this research, we used the discrete element code, flat jointed bonded particle model (Potyondy, 2012) to investigate the measured bi-modularity in rock. The micro rock parameters examined are: inter-granular bond strength; initial micro-fracture present in the sample; and the inter-granular bond stiffness. Also, the impact of bi-modularity on the crack initiation stress (Brace et al., 1966) in rock has been examined. Nicksiar & Martin (2014) investigated the effect of grain size, size distribution and heterogeneity of mineral grains on the crack initiation in crystalline rock and found that those parameters have a minor effect on the ratio of crack initiation stress to the uniaxial compressive strength (UCS). By increasing the grain interlocking, Scholtès & Donzé (2013) could increase the crack initiation of Lac du Bonnet to around 30% of UCS while its value in the lab is approximately 45%.



Figure 1. Ratio of tensile (E₁) and comp. (E_c) modulus of rocks from the literature (Patel & Martin, 2018).

The following sections describe the flat jointed bonded particle model, its calibration, the materials investigated and the impact of micro parameters on bi-modularity and the tensile and compressive behavior observed in the laboratory.

2 FLAT JOINTED BONDED PARTICLE MODEL

The latest development in contact modelling to simulate rock behavior is the flat joint (FJ) model proposed by Potyondy (2012). As shown in Figure 2a and b, in the FJ model, the mineral grains are represented by rigid disks and the contacts by FJs. The FJ contacts are further discretized along as shown in Figure 2c. Each discretized element in FJ fails separately when either the tensile or shear stress exceeds its strength.



Figure 2. (a) 54 mm wide PFC2D FJ contact model with 2998 grains and 14062 FJ contacts (b) grains represented by the disks and flat joints, yellow (c) the discretized FJ contact between the grains.

The parameters for the grains (disks) and contacts are listed in Table 1. These are micro parameters and are impossible to determine from the laboratory tests directly. So, they are obtained by the calibration of macro-parameters like tensile strength, UCS, triaxial strength, and Young's modulus and Poisson's ratio obtained from the laboratory tests. An iterative method is used to find a set of parameters with which the model can produce the properties obtained by the rock in the laboratory.

3 ROCKS INVESTIGATED

In this study, the mechanical properties of LdB granite (Martin, 1993) and Yellow Sandstone has been used (Wei et al., 2021, Yang et al., 2020). Low-porous, crystalline Lac du Bonnet granite has a grain size of 3 to 7 mm. Yellow sandstone has a medium grain size with initial micro-cracks and pores, Figure 3b. The UCS of Lac du Bonnet granite and Yellow Sandstone are approximately 220 MPa and 67 MPa respectively. The moduli ratio for LdB granite (Patel & Martin, 2018) and Yellow Sandstone (Wei et al., 2021) are approximately 0.65 and 0.33 respectively. The shape of mineral grains and initial micro-cracks in an intact sample of Lac du Bonnet granite and Yellow Sandstone are shown in Figure 3 (a) and Figure 3 (b) respectively.



Figure 3. SEM image of an intact (a) LdB granite sample showing complex mineral grains and stress released micro fractures (Patel & Martin, 2018) (b) Yellow sandstone with pores and grains (Yang et al., 2020).

4 CALIBRATION OF THE LABORATORY PROPERTIES

One of the most important issues to consider in the DEM modelling is the rock microstructure. As suggested by (Brown, 1981), the width of the rock sample should be at least 10 times the largest mineral grain present in the rock. Similarly, the ISRM Suggested Method for obtaining the deformability of rock materials in uniaxial compression (Bieniawski & Bernede, 1979) recommends the diameter of the sample should be at least NX (54 mm) size. So, by considering both the above conditions and to mimic intra granular fracture, we chose an average of 50 particles along the diameter. The numerical sample in a UCS test is loaded through frictionless platens. So, a L/D ratio of 1 as suggested by (Potyondy, 2018). The loading rate during UCS and tensile was slow enough to insure a quasi-static response to represent laboratory loading conditions.

The micro parameters of the model were obtained from the calibration of macro parameters from the laboratory tests. This was done using an iterative procedure. The final set of micro parameters obtained which produced acceptable results are shown in Table 1. The macro parameters obtained for the numerical samples are compared with the laboratory results in Table 2. The strength values and the Ec was found to be within 3% of the lab results. While the numerical samples did not show any bi-modularity (Et/Ec~1.0). So, the impact of micro properties on bi-modularity is examined in the next section.

Parameter		LdB Granite	Yellow sandstone
Number of particles along the diameter		50	50
Particle-size ratio		1.5	1.5
Particle modulus	[GPa]	41.0	4.3
Particle stiffness ratio		1.5	1.5
Particle friction coefficient		0.4	0.4
Modulus of FJ	[GPa]	41.0	4.3
Stiffness ratio FJ		1.5	1.5
Bond tensile-strength distribution FJ	[MPa]	15.97	3.66
Bond cohesion FJ	[MPa]	48.0	12.0
Bond friction angle FJ	Degree	35	40

Table 1. List of micro properties obtained after calibration (Parameters are described by Potyondy (2017)).

Table 2. Comparison of macro properties obtained from Laboratory testing and PFC2D (using the micro properties from Table 1).

Rock		Lab (LdB granite)	PFC2D (LdB granite)	Lab (Yellow	PFC2D (Yellow
				Sandstone)	Sandstone)
σ_t	[MPa]	10.6	10.6	3.95	3.56
UCS	[MPa]	224.4	226.2	67.33	67.33
Ec	[GPa]	70.5	72.4	7.79	7.98
E_t/E_c		0.65	0.99	0.33	1.0

5 IMPACT OF MICRO PROPERTIES ON BI-MODULARITY

To investigate the impact of micro properties on the modular ratio of LdB Granite and yellow sandstone the inter-granular bond strength; inter-granular bond stiffness; and initial micro fracture present in the numerical samples were varied for the calibrated samples. By changing the tensile bond strength of numerical Lac du Bonnet granite and yellow sandstone from 15.97 MPa to 7.895 MPa and 3.6 MPa to 2.0 MPa respectively, however, the value of Et/Ec remained constant for both LdB granite and yellow sandstone. As the calibrated bond strengths are different, the normalized plots for Et/Ec with bond strength for both the rocks are shown in Figure 4a.

It was found that bond strength plays a role only after rock fracture not in the elastic zone. Similarly, by changing the bond stiffness of Lac du Bonnet granite and yellow sandstone from 41 GPa to 20.5 GPa and 4.3 GPa to 2.3 GPa respectively, the value of Et/Ec is almost constant at 1.0 for both LdB granite and yellow sandstone Figure 4b. If the bond stiffness is changed for the mineral grains, it will equally impact the stress-strain curve in both compression and in tension keeping the ratio of Ec and Et constant.

The model shown in Figure 2 has 14062 FJ contacts. We inserted microfractures in the model similar to the rocks in Figure 3, by assigning a few percent of these FJ to be broken (slit, Potyondy, 2017), i.e., the FJ contacts are touching but have no tensile strength. The microfracture percentage was then increased. With the increase in microfracture percentage, we found out that the Et value of the numerical sample gradually decreases. Also, the UCS and the tensile strength value of the rock were reduced. The only parameter it did not significantly impact is the Ec. The results for Et/Ec with different microfractures is shown in Figure 4c. With the increase in microfractures the ratio Et/Ec was found to decrease from 0.99 to 0.65 and 1.0 to 0.33 respectively for LdB granite and yellow sandstone. These values match with Et/Ec value observed in the laboratory. In compression, some of the fractures are closed and these closed fractures do not significantly reduce the value of Ec. However, in tension, the fractures have no contact stiffness which reduces the value of Et significantly decreasing Et/Ec.



Figure 4. Results of the numerical analysis for LdB granite and yellow sandstone (YSST) for (a) Ec/Et vs normalized bond strength (b) Ec/Et vs normalized bond stiffness (c) Ec/Et vs ratio of initial bonded to nonbonded contact present in the model.

6 IMPACT OF BI-MODULARITY ON CRACK INITIATION STRESS

Researcher have identified that the crack initiation in rocks is a common phenomenon which occurs around 40% of the UCS (Brace et al., 1966). However, with the micro properties presented in Table 1, the crack initiation was found out to be only 29% and 27.8% of UCS for LdB granite and sandstone respectively, although the models are calibrated to both the direct tensile strength and UCS.



Figure 5. PFC2D results showing the impact of bi-modularity on crack initiation stress on LdB granite: number of cracks formed in an UCS test with increase in axial stress.

To examine the impact of micro-fractures, present in the rock, the model discussed in previous section (with initial micro fracture) was re-calibrated to the UCS and the tensile strength. Figure 5 shows the crack formation with the increase in axial strain for numerical sample with microfractures for LdB granite. Because of the lower value of E_t the model with bi-modularity (25% fracture inside the sample) can take more lateral extension between the mineral grains and delay the crack initiation. Hence, the crack initiation stress is increased from 29% to 41% of the UCS. Similar to LdB granite, crack initiation stress for yellow sandstone was increased to 44.8% of UCS compared to 27.8%.

7 CONCLUSION

To obtain insight into the bi-modularity behavior observed in the laboratory tests on rocks, the DEM code with the flat jointed bonded particle model was used in this research. The effect of bond strength; bond stiffness; and initial microfracture present in the rock were examined for LdB granite

and yellow sandstone. In these studies, when changing one of the above micro material parameters, others are kept constant to see its impact on material behavior. We observed that when the micro fractures in the material in a rock sample increase, the average strength parameters and the tensile Young's modulus of the material decreases. However, it has a small impact on the compressive Young's modulus of the material. When material with 0% micro fracture is compared with the 35% micro fracture, we found that the ratio between the tensile and compressive Young's modulus was reduced from 1.0 to 0.65 for LdB granite and 1.0 to 0.33 with 44% microfractures for yellow sandstone (values observed in laboratory). Micro fractures in the rock when loaded in compression have only a minor impact on the overall Young's modulus. However, the same microcracks when open by tensile stresses reduce the Young's modulus of the material. Only by incorporating the bimodularity in the material, the crack initiation stress increased to 41% and 44.8% of the UCS for LdB granite and yellow sandstone. These values were found close to the value observed in laboratory. With a lower value of tensile Young's modulus, the sample can take more lateral extension between the mineral grains and delay the crack initiation. Inter molecular bond strength and bond stiffness found to have no impact on bi-modularity of rock.

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