Study on the characterization of rock heterogeneity and simulation of fracture process based on the mesoscopic structure

ZHANG Yanbo$^{1,2}$, ZHANG Enyuan$^{1,2,*}$, YAO Xulong$^{1,2}$, LIANG Peng$^{1,2}$, TIAN Baozhu$^{1,2}$, SUN Lin$^{1,2}$, LIU Xiangxin$^{1,2}$, WANG Shuai$^{1,2}$

$^1$ College of Mining Engineering, North China University of Science and Technology, Tangshan, Hebei 063210, China; $^2$ Mining Development and Technology Safety Key Laboratory of Hebei Province, North China University of Science and Technology, Tangshan, Hebei 063210, China

*Corresponding Author: zey950815@163.com

Abstract. This study aims to explore the effect of rock heterogeneity caused by meso-structure differences on the macro-mechanical properties and fracture evolution process. With the help of computed tomography, the meso-structure characteristics of coarse-grained red sandstone are obtained, starting from the meso-structure level. The digital characterization of heterogeneous rocks is completed with the use of image-processing methods, and a rock equivalent crystalline model is constructed. A numerical simulation study is performed with the particle flow PFC$^{3D}$ 5.0 program. The results show that (1) the main form of rock heterogeneity is a meso-structure difference, and this determines the rock’s macro-mechanical properties and failure characteristics. The meso-structure difference mainly plays a role in the post-peak damage weakening stage of rock, and the slight difference leads to damage in different development modes. (2) The crack initiation starts at the cemented and crystalline grid surfaces, which is randomly distributed. The crack evolution process is selective and affected by the types and distribution of the surrounding mineral particles. The development of cracks is dominated by secondary cracks, distributed in strips, in the area of mineral particles with strong mechanical properties. In contrast, cracks are densely developed and spread around in a cluster in the area of mineral particles with weak mechanical properties.

Key words: heterogeneity; image processing; meso-structure; numerical simulation

1. Introduction

Rock is a non-uniform, multi-phase brittle material. One of its basic characteristics is the heterogeneity, and under external forces, it is also the main reason for the non-uniformity and non-linearity of rock’s physical and mechanical properties [1-2]. Under the external load and different mechanical responses, the difference in complex geometry, distribution, and physical and mechanical characteristics of the different meso-structures leads to the uneven stress and strain field distribution.

There are mainly two methods for characterizing rock heterogeneity according to the research results of many scholars. (1) To virtually generate three-dimensional (3D) material structures, the use of statistical methods to describe the heterogeneity of rocks [3-4], such as Monte Carlo or stochastic
methods, is recommended, assuming that the mechanical parameters of rock elements follow Weibull distribution [5-7]. However, using statistical methods cannot truly reflect the internal structure of materials [8]. The structure and mesoscopic composition of the internal granular material determine the macro-mechanical properties, especially for rock materials, and the contact of the contours of different internal particles will affect the final macro-damage mechanism; therefore, this kind of method also has relatively large limitations. (2) Considering the heterogeneity of rock microstructure based on digital image-processing methods, Zhong-qi et al. [8-10] used digital image-processing technology and numerical methods such as finite element method and finite difference method. To study the influence of microstructure of geotechnical engineering material on its internal stress distribution, we combined these methods. To study the influence of the heterogeneity caused by the meso-structure on the stress distribution and crack propagation of the model, Lan et al. [11] used Universal Distinct Element Code. This kind of method considers the real structure of the internal rock material as much as possible and can establish a refined numerical model. It has been widely used in the numerical calculation of geotechnical engineering materials recently.

The key to further research on rock heterogeneity lies in whether it can accurately describe and characterize the uneven microstructure of the rock. Rock failure and instability are a cross-scale evolution process from meso-scale to macro-scale. It is difficult to obtain the meso-structure of the rock by conventional means as experimental methods are limited. The scanning accuracy can reflect the internal microstructure of the material well through the rapid development of computed tomography (CT) technology [12]. The progress made by some scholars in the digital characterization of the meso-structure of materials [13-15] also provides a basis for the construction of 3D digital and vectorized structural models of materials.

In summary, to obtain the internal microstructure of coarse-grained red sandstone, this study used the industrial micro-CT system, completed the identification and extraction of the microstructure through digital image-processing technology, and constructed a rock equivalent crystalline model. The uniaxial compression simulation test was conducted to study the effect of rock heterogeneity caused by meso-structure on the macro-mechanical properties and crack evolution process, combined with the particle flow PFC3D 5.0 program.

2. Specimen preparation and CT scan

2.1. Rock ore appraisal

The CT scan used a coarse-grained red sandstone specimen (Figure 1a). The specimen is a cuboid specimen with a size of 50 mm × 50 mm × 100 mm. This type of red sandstone comprises detrital particles and interstitial materials identified under a polarized light microscope. The cementation method used is pore cementation, and the detrital particles are primarily quartz, feldspar, mica, and rock debris. The size of debris particles is generally 0.25–0.5 mm (medium sand), partly 0.5–2 mm (coarse sand), a few are 0.06–0.25 mm (fine sand), and some are 2–8 mm (fine gravel ±25%). The debris particles are mostly sub-angular, some are sub-circular, and the sorting was poor (see Figure 1b for details).

![Figure 1](image1.png)

**Figure 1** Original rock specimen and rock ore identification: (a) Rock specimen, (b) Orthogonal polarized light picture

2.2. CT scan
Using Phoenix V|tome|xm industrial CT produced by General Electric Company of Germany, the CT scanning of the mesoscopic structure of the rock specimen was completed at the Analysis and Testing Center of the North China University of Science and Technology, and its micron focus detail resolution ability was ≤2 μm and nano-focus detail resolution was ≤0.5 μm. The red sandstone reconstruction model was obtained using VGStudio Max software after the specimen was scanned, as shown in Figure 2c.

![CT scan](a) Industrial CT, (b) Original rock specimen, (c) Refactoring model

3. Image processing and construction of digital rock model

3.1. CT image analysis and processing

On CT images, the lower the density, the darker the color; the higher the density, the brighter the color. The main component of coarse-grained red sandstone is considered to be a sandstone matrix with a density of 2.74 g/cm³, considering that its internal composition is relatively complex, and the basic mineral composition is mica, quartz, feldspar, and clay minerals. The density of mica, feldspar, and quartz are 2.7–3.3, 2.54–2.61, and 2.65 g/cm³, respectively, according to the mineralogical analysis. In this study, the density of clay mineral is 1.7 g/cm³.

The brightest color is mica mineral, the darkest is clay mineral, and the sandstone matrix, quartz, and feldspar are medium in color, according to the color characteristics of CT images. The color characteristics of mica and clay minerals are more obvious, but the color boundary between the sandstone matrix and the quartz and feldspar minerals is not very obvious.

This study, therefore, used pseudo-color conversion on CT slice images and completed the identification and extraction of components in the category of color in the HIS color space. The slice after pseudo-color conversion is shown in Figure 3b, and the result of material component identification and extraction is presented in Figure 3d. Binarization and median filtering were also performed considering the needs of subsequent digital modeling, and the final processing result is provided in Figure 3c.

![Image processing](a) The original image, (b) Pseudo color processing, (c) Component identification and extraction, (d) Binarization, (e) Median filtering

3.2. Construction of rock heterogeneous model

The two-dimensional information in the picture needs to be converted into vectorized data required for modeling to construct a heterogeneous rock model. The digital image comprises pixels, and each pixel represents a small square area. Rock is a continuous solid material. It is assumed that the CT slice image can represent the microscopic structure of the material with a very small thickness (t) in the reconstruction process, so the square grid corresponding to each pixel can be extended in the depth direction in parallel to t and thus can be converted into a 3D cuboid grid that can characterize the meso-structure. If t is small, the error is negligible.
We divided the whole rock into eight pieces and built a local model in turn. Heterogeneity was manifested by the differences of the meso-structures within each model. The CT image resolution was reduced to 80 × 80 pixels limited by the computer’s capability. The actual side length of the specimen was 50 × 50 mm. The actual area was therefore represented by one pixel (0.39 mm²). Eight sets of local heterogeneous characterization models with different mineral contents and distribution forms were constructed based on the aforementioned principles and methods. As shown in Figure 4, the model size was the same as the indoor test sample.

| Number | Quartz/% | Feldspar/% | Mica/% | Sandstone matrix/% | Clay/% |
|--------|----------|------------|--------|-------------------|-------|
| Sample 1 | 0.36     | 8.99       | 0.41   | 52.82             | 37.43 |
| Sample 2 | 0.31     | 8.20       | 0.26   | 58.52             | 32.71 |
| Sample 3 | 0.81     | 25.06      | 0.31   | 53.45             | 19.94 |
| Sample 4 | 0.86     | 20.49      | 0.41   | 58.30             | 19.32 |
| Sample 5 | 1.08     | 21.90      | 0.35   | 57.35             | 19.32 |
| Sample 6 | 0.95     | 18.85      | 0.15   | 59.30             | 20.75 |
| Sample 7 | 0.86     | 22.13      | 0.27   | 51.37             | 25.37 |
| Sample 8 | 1.07     | 21.34      | 0.33   | 56.85             | 20.42 |

4. Grain based modeling and particle flow simulation

4.1. GBM model and its construction

Grain-based modeling (GBM) is a characterization model based on the particle flow program, which comprises a large number of rupturable polygonal crystal particles. The GBM model can effectively conduct rock mechanical behavior research from the meso view, as proposed by Potyondy [16] and Zhou [17]. The construction process of the GBM model of this study is shown in Figure 5.

![Figure 4 Heterogeneous rock sample construction](image)

![Table 1 Component content of each rock sample](table)

![Figure 5 The construction process of GBM](image)
mechanical parameters of materials in this study are shown in Table 2. The meso parameters of all component boundaries in the model were set to be consistent for the ease of calculation. Table 3 shows the final meso parameters for calibration.

**Table 2** Macroscopic mechanical parameters of minerals

| Material          | Uniaxial compressive strength /MPa | Modulus of elasticity /GPa | Poisson's ratio | Density /Kg·m³ |
|-------------------|-----------------------------------|---------------------------|----------------|----------------|
| Sandstone matrix  | 46.056                            | 5.826                     | 0.24           | 2740           |
| Quartz            | 705                               | 96                        | 0.08           | 2650           |
| Feldspar          | 396                               | 67                        | 0.27           | 2595           |
| Mica              | 250                               | 40                        | 0.36           | 3150           |
| Clay              | 22.5                              | 6                         | 0.45           | 1700           |

**Table 3** Meso parameters

| Bond model          | Material          | Parameters |
|---------------------|-------------------|------------|
|                     |                   | E_mod/GPa | P_b_mod/GPa | K_ratio | P_b_ten/MPa | P_b_coh/MPa | P_b_fa |
| Linearparallel      | Sandstone matrix  | 0.93       | 3.84        | 6.71    | 10.07       | 5.04        | 20     |
| Bond Model          | Quartz            | 15.21      | 37.77       | 1.26    | 64.85       | 64.85       | 51     |
|                      | Feldspar          | 13.51      | 35.62       | 4.36    | 59.1        | 59.1        | 36     |
|                      | Mica              | 7.83       | 22.91       | 5.47    | 41.52       | 41.52       | 28     |
|                      | Clay              | 1          | 4           | 8.05    | 4.70        | 4.70        | 15     |
| Smooth-joint        | Material boundary | 716.63     | 367         | 2.26    | 1.75        | 1.75        | 18     |

4.3. Load simulation

The sample was loaded by the wall movement, given the constant velocity of 0.1 m/s at both ends of the wall. The loading was stopped when the stress value dropped to 70% of the peak stress value. The crack had propagated to an obvious observation stage at this time, and the test was ended.

5. Analysis of test results

5.1. Analysis of mechanical properties and macroscopic failure modes

The stress–strain curves of the whole process of eight groups of rock samples under uniaxial compression are shown in Figure 6. The stress–strain curves of the eight groups of rock samples coincided in the elastic phase before the peak, whereas there were obvious fluctuations in the elastoplastic and post-peak failure phases. The difference between the maximum value and the minimum value was 4.02 MPa, which was 16.14% of the average compressive strength. The average value of uniaxial compressive strength was 24.9 MPa. The difference between the maximum value and the minimum value was 0.57 GPa, which was 13.15% of the average elastic modulus, and the average value of the elastic modulus was 4.35 GPa. It can be seen from the final failure morphology maps of the eight groups of samples (Figure 7) that the failure modes of samples 3, 5, 6, and 8 were mainly a tensile splitting failure, and the failure modes of samples 1, 2, and 4 and 7 were primarily a shear failure.

The mineral contents inside the rock samples 1, 5, and 8 were the same as can be seen in Table 1; however, they showed different mechanical characteristics and failure modes. The fracture development methods were different, although the failure modes of rock samples 1 and 5 were the same. The difference between the rock samples was mainly the distribution of the meso-structure according to the construction method of the Section 3.2 rock sample. Hence, it is shown that the difference in the meso-structure distribution had no obvious effect on the linear elastic stage and had a significant effect on the elastoplastic and post-peak failure stages. This point also demonstrates that the small differences in the
meso-structure will lead to very different damage development modes, which will lead to differences in macroscopic mechanical properties and damage characteristics, and that the elastoplastic stage and the post-peak failure stage are unstable (Figure 8).

Figure 6 Stress-Strain Curves of Uniaxial Tests

Figure 7 Macroscopic failure pattern: (a) Sample 1, (b) Sample 2, (c) Sample 3, (d) Sample 4, (e) Sample 5, (f) Sample 6, (g) Sample 7, (h) Sample 8

5.2. Analysis of microscopic damage characteristics

Take Sample 3 as an example. It can be seen that the cracks first appeared in the interface between the particle interface and the crystalline grid surface from the process of crack development and evolution (Figure 9) and were dispersed in the specimen, mainly stretching and intergranular cracks. At this stage, the number of fissures maintained steady growth. The failure points near each other began to connect as the load increased, forming multiple small-scale crack concentration zones, primarily around weak (soft) mineral particles such as clay minerals and sandstone matrix. The model as a whole began to enter the yield stage when the stress was close to 80% of the peak value. The cracks in different regions began to penetrate gradually at this time, the main crack zone was initially formed, and the cracks began to grow and expand rapidly. Transgranular tensile cracks were generated inside it due to the relatively low strength of the weak mineral crystallites. The rapid increase in the number of intergranular cracks was because the intergranular bonding strength was smaller than the internal strength of the crystal particles. Therefore, expansion along the crystal boundary was preferred in the process of crack expansion. The number of cracks began to increase sharply when the stress reached the peak strength point. The cracks in different regions along the loading axis started to interpenetrate and developed to form the final main crack. At this time, the growth rate of transgranular shear cracks was the fastest, which were primarily distributed inside the crystal body where the surrounding structural surface was fractured and dislocated, especially inside the weak mineral crystal body with weak mechanical properties. The main reason for the rapid expansion and penetration of transgranular fracture was the local uneven stress distribution. Local instability evolved into macro-fractures in the post-peak period, and the cracks generated by the failure of the smooth joint model in the direction of the loading axis ran through, resulting in the macro-fracture of the rock along the axial direction.

The evolution of the main crack zone was consistent with the distribution of weak mineral particles. Generally, it developed along with the distribution of clay particles and sandstone matrix particles judging from the distribution position of the primary and secondary crack zones. The number of secondary crack zones was relatively small, mainly distributed around strong mineral particles, and gradually developed outward along the crystalline grid, and the shape was mostly strip-shaped. The crack development evolution was influenced by the types and distribution of surrounding mineral
particles and was selective from the perspective of the evolution process of crack development at different cross-sectional locations. For example, at the 8 mm cross-section, the main cracks developed slowly at the early stage of development due to the blockage of strong mineral particles such as feldspar and failed to form a more obvious main crack zone. The secondary crack derivation time node was advanced, well-developed, obviously more than 42 mm cross-section, and widely distributed.

![Figure 8](image1)

**Figure 8** Axial Stress (Crack Growth) - Strain Curves of Uniaxial Tests of sample 3

![Figure 9](image2)

**Figure 9** Evolution of cracks in different cross-sectional areas of sample 3: (a) 42mm section, (b) 8mm section

6. Conclusion
The following conclusions were drawn from the results.

1. The physical state of the rock can be digitized using CT. Combined with image-processing methods, the meso-structure information of the rock can be attained, and a numerical model can be established to characterize the meso-structure of the rock, which provides a feasible method for further study of the meso-mechanics of the rock.

2. The meso-structure difference is the main form of rock heterogeneity, and it determines the rock’s macro-mechanical properties and failure characteristics. The meso-structure difference mainly plays a role in the post-peak damage weakening stage, and the slight difference in the meso-structure will lead to a completely different damage development mode.

3. The crack initiation starts at the cemented surface and crystalline grid surface, which is random in distribution. The crack evolution process is affected by the types and distribution of the surrounding mineral particles and will be selective. The development of cracks is dominated by secondary cracks distributed in strips in the area of mineral particles with strong mechanical properties. In the area of mineral particles with weak mechanical properties, cracks are relatively densely developed and spread around in a cluster.
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