Research Article

3D XCT Mesostructure Characterization and Image-Based Discrete Element (DE) Modelling of Failure Patterns in Coal Gangue Particles (CGPs)

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The paper presents an application of milli- and micro-XCT to mesostructure characterization of CGPs and failure patterns analysis using dynamic impact simulations. In this study, XCT scanning experiments are firstly conducted on CGPs, followed by a series of image analyses with qualitative results. Then, the 3D mesomorphological parameters and internal composition of individual particles are quantitatively characterized. Finally, dynamic impact loading in y-axis direction is modelled to investigate the 3D mesostructure and different impact velocity effects on failure patterns of individual particles. The studies show that the mesomorphological parameters present different distribution characteristics in individual CGPs. The approximate location of gangue phase is the key parameter that should be taken into account to study failure patterns as well as fracture mechanism of the heterogeneous rock materials. The XCT image-based numerical model proved to be an effective tool that gives insights into the mesodeformation mechanisms of heterogeneous coal rock (HCR) undergoing dynamic impact failure behavior.

1. Introduction

Multiscale experiments and modelling of multiphase mineral materials, such as coal, gangue, and various composite materials, are of critical importance for the detailed analysis of the mesostructure and failure patterns of coal ores. In general, the crushing performance for CGPs depends on the statistical characteristics of geometric shape and mesostructures, such as internal composition distribution, phase continuity, and initial damage. Currently, research studies on the characterization of morphological and mechanical properties of individual CGPs are mainly based on experimental analysis [1–4]. Although the experimental method could provide statistic results, unavoidable sampling errors are widely existed by using experimental analysis. Especially, the geometric shape and mesostructure characteristics of individual particles are the determinant of their fragmentation characteristics. Therefore, it is important to link the crushing performances for CGPs to their complex mesostructures.

Qualitative and quantitative analyses of the mesostructure characteristics and mesocrack evolution mechanism will lead to more accurate descriptions and thus improvement to the crushing process [5]. Two-dimensional mesoscale finite element models with realistic mesostructure of concrete are developed using micro-XCT images to simulate complex nonlinear fracture [6, 7]. The microstructural characteristics of asphalt mixture under different compaction powers are investigated [8, 9]. Physical and hydraulic properties of a coastal sand aquifer were derived using micro- and macro-X-ray computed tomography (XCT) techniques [10, 11]. The copper and iron ores were crushed using a jaw crusher first, and then the products were evaluated for particle damage and copper grain exposure by X-ray computed tomography [12, 13]. A finite element model...
model of coke was generated using micro-X-ray CT, and coke strength was numerically evaluated using its microstructure [14]. The principle, the advantages, and the limitations of XCT itself are presented, together with an overview of some current applications of micro-CT in geomaterials [15–19].

Characterization of multiphase mineral using XCT techniques would be extremely helpful for an improved understanding of coal particle crushing processes. Novel image processing techniques combined with stochastic analysis are also used to analyze the 3D images of the porous structure of coal [20]. The fraction of mineral exposed and the ultimate recovery for a given particle size distribution can be established by X-ray microtomography [21]. The characterization of individual multiphase particle has been studied by Arias and Miller [22], and several effective algorithms were also proposed by Miller and Lin to study the mesostructure of different minerals [23–25]. From the abovementioned analysis, most of the studies have investigated the mesostructure of individual particles, but only a small number of coal gangue samples have been studied by the very limited XCT scanning studies and the results are inconclusive. Besides, the inclusions in individual particles are usually assumed to be a polygonal irregular body, which has huge difference with the real internal mesostructure in individual CGPs. This may also lead to theoretical and numerical models that cannot study the fracture characteristics of individual CGPs inaccurately.

In this study, we aim to improve the understanding of mesomorphologies of CGPs (such as geometric shape, 3D mesomorphological parameters, and internal composition) and their correlations with loading conditions, combining the micro-XCT scanning tests and numerical simulations. A large number of raw coal gangue samples with different internal mesostructures are examined in detail using different image processing techniques. A reliable 3D mesoscopic numerical approach (the image-based DE model) is also proposed to study 3D fracture evolution process of HCR under different impact velocities at the mesoscale.

2. XCT Image Acquisition, Processing, and Analysis

2.1. XCT Scanning. The packed crushed CGPs with particle size range from 10–100 mm, which were provided by Dengfeng mining in China, are simply packed in a cylindrical container (Figure 1(a)) and scanned on Philips mili-CT equipment (Figure 1(b)). The 3D image data obtained from Philips mili-CT equipment contain 901 projections of 512 × 512 pixels with a voxel resolution of 470 μm. Another micro-XCT-400 machine with much higher resolution (Figure 1(c)) is used to scan the fine particles with size 1–5 mm [26]. Figures 1(d) and 1(e) show the sample container with a diameter of 40 mm and 5 mm, respectively. These fine samples are tightly packed in the containers to obtain higher quality images with voxel size 32 μm for subsequent data analyses.

Figure 2 shows the variation of CT values of the sectioned 2D images along the probeline AB. The sensitivity to location was examined by using line probe to verify that most of CGPs are multiphase particles. As shown in Figure 2, different mineral phases are clearly distinguished in different grey scale levels. The dark grey, light grey, and light white regions represent sections of coal, gangue, and pyrite mineral grains, respectively. These raw CT images are then processed and analyzed to acquire the quantitative information to characterize the 3D mesostructure of individual CGPs.

2.2. CT Image Processing and Segmentation. A series of image processing procedures, including image denoising and image enhancing, should be applied to original CT images that aim to increase the precision of subsequent processing algorithms. It is clear that segmentation is one of the most critical steps to obtain accurate morphological parameters in the process of boundary regions between particle phases and cracks. For quantitatively analyzing particle damage accurately, segmentation of the particle phases and cracks from the background is accomplished by the conventional threshold algorithm or feature-based classification algorithm [27, 28], depending on the different particle phases and crack characteristics in particles. The conventional threshold segmentation algorithm works well for most coarse coal gangue particles, due to the high-contrast boundaries in internal particles and sufficient scanning resolutions. However, for a fine particle image with a scale parameter (i.e., the ratio of particle size and voxel size [28]) less than 30 (Figure 3(a)) or artificial CT images (Figure 3(d)), the conventional threshold often provides unsatisfactory results because of some noises similar to our interest regions and the insufficient contrast boundaries, as shown in Figures 3(b) and 3(e), where the segmented image is not satisfactory for detailed analysis of internal compositions and internal damages. Correctly identifying internal composition and internal damage in particles by XCT can be challenging, due to insufficient contrast boundaries or small characteristics near the resolution limit.

In this regard, a feature-based classification method, which not only takes image intensities but also a series of image features into account to identify particle boundaries [29], is proposed to extract useful features to realize better segmentation effect [30]. Firstly, red and green lines are annotated as the training set of the particle phase and background, respectively (Figure 4(a)). Then, the random classifier was trained from the selected data, and the particles’ extraction image and background image are shown in Figures 4(b) and 4(c), respectively. Finally, the improved segmentation results of the small-scale image and artificial CT image are shown in Figures 3(c) and 3(f), respectively. It proved that the feature-based classification method is a powerful tool to improve the accuracy of the specific image.

Similarly, different mineral phases and background regions are selected as a training set to segment different mineral phases from the background (air). The improved segmentation results for the small-scale image and artificial CT image shown in Figure 5 are satisfactory for subsequent segmentation process and for detailed quantitative analysis.
of multiphase particles. Table 1 shows the comparative results of composite analysis for different algorithms. As shown in Table 1, the feature-based segmentation algorithm has been found to perform very well in the analysis of small-scale images of CGPs. In fact, for the small-scale image of CGPs (scale parameter 28), the precision difference between the two algorithms can reach to 28.08% when traditional image segmentation was replaced by feature-based segmentation. For the artificial image of CGPs (scale parameter 84), the range of error was 6.34% when traditional image segmentation was replaced by feature-based segmentation.

3. **3D Individual Particle Characterization Using XCT**

3.1. **Internal Composition Characterization of Individual CGPs.** Intensity histograms of the randomly selected ten particles are shown in Figure 6. It is clear from Figure 6 that
the intensity characteristics of individual particles show different distribution characteristics, and a higher density mineral phase has a higher intensity value. The intensity-frequency distribution curve of the multiphase particle shows multipeak characteristics. Further analysis validated that individual CGPs can be divided into three types: single-phase particle, biphase particle, and triphase particle. In this regard, three typical particles were selected and their intensity histograms were determined, respectively, to illustrate the difference of individual particles. Frequency distribution curves and 3D volume-rendering images are shown in Figures 7–9, respectively.

Intensity-frequency distribution curves and 3D volume-rendering images of the selected single-phase particles are shown in Figures 7(a) and 7(b), respectively. It is clear that the intensity histograms of individual CGPs are fitted well using the normal distribution model. The coal intensity histogram varies from 0 to 450, and its peak value is 315. For
a gangue particle, the intensity histogram varies from 1200 to 2400, and its peak value is 1763. The intensity histogram of the gangue particle has only one peak, which further indicates that the selected gangue particle is a single-phase mineral. It can also be concluded from Figure 7 that big difference exists between the intensity histogram distribution of coal and gangue, which can be distinguished from the intensity histogram easily.

Figure 8 shows the results of the intensity-frequency distribution curve and the 3D volume-rendering image of
the selected biphase particles. As indicated from the curves shown in Figure 8, the intensity value varies from 100 to 2100, and the frequency distribution curve of intensity has two peaks, which indicated that the selected particle is a biphase particle (the individual particles are composited by coal and gangue, respectively). The intensity histogram of biphase particle is analyzed through multinormal distribution. It can be seen that the experimental data fit well, relating the frequency distribution and the intensity values. Further analysis shows that the volume proportion distributions of coal and gangue are 82.91% and 17.09%, respectively.

Figure 9 shows the intensity histogram and volume rendering of the selected triphase particle. The intensity histogram presents a trimodal distribution, and the intensity value varies from 120 to 3100. The peak value of three phases can reach to 710, 1500, and 3078, respectively. The volume proportion distributions of coal, gangue, and pyrite are 23.27%, 41.58%, and 35.15%, respectively.
3.2. Characterization of 3D Mesomorphological Parameters.
In order to illustrate internal damage of the individual CGPs, the original CT image of the selected coal particle shown in Figure 10(a) is typically segmented and reconstructed (Figure 10(b)) from the packed particle bed. It is clear that cracks in different slices and internal damage can be clearly identified from original CT images. These raw coal CT images are processed using different segmentation algorithms to get the satisfied binary images shown in Figure 11. As shown in Figure 11, the cracks shown in black are extracted in different slices, and the particle boundary is marked in grey color. The segmented CT images provide quantitative information to characterize internal damage of individual particles, and the quantitative analysis results can be seen in Table 2. The calculation indexes shown in Table 2 were described in [31–34]. It is clear that different mesomorphological parameters (crack number, length, width, perimeter, area, and angle) can be obtained in different slices. The variation tendency of the fracture ratio in different slices of the selected individual particle is shown in Figure 12. As shown in Figure 12, there are two peaks during slices 7~15 and 45~62, which indicates that fracture degree of the coal particle is relatively serious in these two parts. It is also clear from Figure 12 that different slices have different fracture ratios, which indicates that different damage degrees are existed in internal particles. Further 3D quantitative analysis showed that the fracture ratio can reach to 5.06%.

From the abovementioned analysis, it proved that the mesostructure of individual CGPs can be qualitative and quantitative analyzed after loading (i.e., volume fractions, sizes, shapes, and spatial distribution of mineral phases). Due to the impact loading process always occurs within a few microseconds, the continuous investigations of the entire fracture process with the current XCT techniques is not workable for technical reasons yet. In this regard, the 3D numerical image-based DE model provides a feasible way to examine the mesostructure damage and fracture evolution, which is described in detail in the following section.

4. XCT Image-Based DE Simulations

4.1. 3D Image-Based DE Model Generation. A coal cube specimen of size 32 mm (Figure 13(a)) was cropped from raw coal 3D dataset of 16 bit float with 1372 slices. For each slice, there are $1720 \times 1771$ pixels of $32 \mu m$ in $x \times y$ direction in the sampled image dataset. To reduce the data processing time, the 3D data size was reduced to 500 MB for the 3D original dataset with the resolution also compressed from $32 \mu m$ to $100 \mu m$ using Avizo software. These raw compressed CT images are segmented to get the 3D mesomorphologies of HCR, and then reconstructed to get the 3D surface model. This is followed by Laplacian smoothing [35] (Figure 13(b)) and surface simplification [36] to get the simplified surface model (Figure 13(c)). As shown in...
There are 36,386 triangles in the simplified surface model.

In the image-based DE modelling process, the total 91,672 discrete elements (balls) with the radius 0.433 mm were put into the simplified surface model to generate the 3D DE model (Figure 13(d)). As shown in Figure 13(d), 77,387 and 14,285 balls were identified as coal and gangue clusters based on the shape of the coal phase and gangue phase, respectively. The followed procedure is the settlement of the balls until their total kinetic energy became insignificant.

In DEM analysis, the macroscale mechanical parameter, such as elastic modulus $E$, Poisson ratio $\mu$, and compressive strength $\sigma$, cannot be directly imposed into the numerical model. Therefore, it is critical to select appropriate mesoparameters for the numerical model that aims to represent the accurate macroscale mechanical behavior of HCR. The calibration approach is used to determine these appropriate mesoparameters, and the detailed calibration procedure [37, 38] has been demonstrated in Figure 14, which is described in detail as follows:
Conduct uniaxial compressive experiments on the selected coal sample to determine the intrinsic material parameters, such as elastic modulus, shear modulus, Poisson’s ratio, and compressive strength.

Establish 3D DE models of HCR in PFC3D.

Conduct uniaxial compression simulations on the 3D DE model of HCRs to determine the meso-mechanical parameters.

LY_xe calculated simulation and experimental parameters were compared, which aims to calibrate the mesoparameters of HCRs. If the simulation results were not consistent with the experimental parameters, a new numerical model should be created by modifying the mesoparameters until the simulation parameters were consistent with the experimental parameters.

With the assumed mesoparameters of the HCR, the DEM calculations provided the uniaxial compressive strength of 8.9 MPa, the compressive elastic modulus of 3.9 GPa, and Poisson ratio of 0.21, similarly as in the standard uniaxial compression experiments of coal rocks ($\sigma = 9.6$ MPa, $E = 4.2$ GPa, and $\mu = 0.23$). The final mesoparameters of the simulation model are shown in Table 3.

Figure 12: Variation tendency of fracture ratio in different slices of individual coal particles (the cracks are in blue and the coal gangue in grey).

Figure 13: 3D DE model generate of HCR. This figure presents (a) the raw coal sample; (b) the smoothed surface model; (c) the simplified surface model; and (d) the 3D DE model of HCR.

Figure 14: Calibration procedures for mesoparameters of HCR.
4.2. Dynamic Impact Simulation. For the simulation, particle flow code in three dimensions (PFC3D) in version 5.0 [39] is selected to run the DE model under dynamic impact loads. Dynamic impact loading in positive $y$-axis directions are modelled to investigate the 3D mesostructure effects on the damage patterns and fracture mechanism under different impact velocities. The 3D DE model of HCR under positive $y$-load is shown in Figure 15. As shown in Figure 15, the top and bottom walls are created to apply the load in positive $y$-direction, where the desired impact velocity corresponding to a certain height $h$ is applied on the top wall and the bottom wall remains fixed, and lateral deformations are allowed freely. To describe the simulation results presented below, the time evolutions of the wall force generated at the HCR-wall interface and the damage ratio [40–42] (i.e., the damage ratio of coal and gangue is defined as the ratio of the number of broken bonds and initial bonds in the coal phase and gangue phase, respectively) are selected as the two important parameters to quantitatively characterize failure patterns and load-carrying capacities.

The impact simulations for HCR have been used to examine how the breakage behaviors are affected by different impact velocities in positive $y$-load mode. It should be noted that the numerical simulation process was ended with the condition of the wall force reaching 60% of the maximum wall force. The wall forces for HCR as functions of the time in $y$-load under different impact velocities are shown in Figure 16, with key loading points (A–D(positive $y$-load)) marked at the curve of wall force under 8 m/s, respectively. As shown in Figure 16, the maximum wall forces of the HCR are calculated to be 69.01, 69.37, 82.33, 87.43, and 83.94 KN in negative $y$-load with the impact velocities of 6, 8, 10, 12, and 14 m/s, respectively, with 17.78% maximum difference. The maximum wall force increased first then slightly decreased, which indicated that there exists an optimal impact velocity with best crushing effects but without excessive energy consumption. Figure 17 compares the damage ratio results of HCR and different mineral phases (coal and gangue, respectively) affected by positive $y$-load under different impact velocities. As shown in Figure 17, the damage ratios of the HCR and coal phase are much higher than the results of the gangue phase in positive $y$-load mode, which indicated that gangue phases are less damaged in the positive $y$-load mode.

The internal damage initiation state and evolution state of the HCR in positive $y$-load are shown in Figure 18. The four key loading points (A–D) in the positive $y$-load mode of the curves at 8 m/s are selected to illustrate how the gangue interface affects initiation and propagation of damage bands. It should be noticed that the fragment color, which are determined by the built-in language FISH provided by PFC3D, mainly caused by the evolution state of HCR. As shown in Figure 18, only few percentage of fine debris is generated at the HCR-wall interface in loading point A. The damage bands tend to propagate from the gangue interface to form several main fragments due to the relative movement between the HCR and the wall, which can be seen in the evolution states from the loading point B to D. It is clear from the evolution images of the key points A–D that the damage initiates mostly around the gangue interface, which leads to generation of several coal fragments mostly around

| Table 3: Mesoparameters of the PBM used in the DE model. |
| Mesoparameters                  | Value | Mesoparameters                  | Value |
| Ball density $\rho_c$ (kg/m$^3$) | 1540  | Ball stiffness ratio $k_y/k_z$   | 2.17  |
| Effective modulus $E^*$ (Pa)     | 2.3e9 | Tensile strength $\sigma_y$ (Pa) | 7.90e6|
| Coal Friction coefficient $f$    | 0.3   | Cohesion $\tau$ (Pa)            | 3.95e6|
| Installation gap $g_y$ (m)       | 1e−4  | Friction angle $\varphi$ (°)    | 28    |
| Radius multiplier $\bar{r}$     | 1     | Normal damping ratio $\beta_{\alpha}$ | 0.75 |
| Ball density $\rho_k$ (kg/m$^3$) | 2950  | Ball stiffness ratio $k_y/k_z$   | 2.582 |
| Effective modulus $E^*$ (Pa)     | 6.0e9 | Tensile strength $\sigma_y$ (Pa) | 3.65e7|
| Gangue Friction coefficient $f$  | 0.3   | Cohesion $\tau$ (Pa)            | 3.04e7|
| Installation gap $g_y$ (m)       | 1e−4  | Friction angle $\varphi$ (°)    | 34    |
| Radius multiplier $\bar{r}$     | 1     | Normal damping ratio $\beta_{\alpha}$ | 0.75 |
| Interfaces Effective modulus $E^*$ (Pa) | 4.15e9 | Tensile strength $\sigma_y$ (Pa) | 3.42e7|
| Friction coefficient $f$         | 0.3   | Cohesion $\tau$ (Pa)            | 1.72e7|
| Installation gap $g_y$ (m)       | 1e−4  | Friction angle $\varphi$ (°)    | 31    |
| Ball stiffness ratio $k_y/k_z$    | 2.38  | Normal damping ratio $\beta_{\alpha}$ | 0.75 |

Figure 15: 3D DE model of HCR generation and in the positive $y$-load mode.
the gangue interface, and only the upper part of the gangue phase is changed to the failure state. It indicated that the damage bands tend to propagate along the gangue interface under the condition of the loading direction, which is almost perpendicular to the growth direction of the gangue interface.

5. Conclusions

This paper presents an application of milli- and micro-XCT to mesostructure characterization of individual CGPs and failure patterns analysis using dynamic impact simulations. A detailed study has been presented on the quantitative computational characterization of the mesostructure of individual CGPs, and the quantitative numerical simulation results are also showed as follows:

(1) The conventional threshold segmentation algorithm and the feature-based classification algorithm are proposed to identify particle boundaries and mineral phase boundaries of CGPs. It proved that the feature-based classification algorithm has good segmentation results of the small-scale CT image and the artificial CT image. The volume proportion distribution of internal composition and initial damage of individual CGPs can be determined through different XCT image analysis methods.

(2) Internal composition and 3D spatial distribution of mineral phases in individual particle can be characterized using XCT techniques. The mesomorphological parameters of individual particles are also carefully quantified using various image processing techniques. All the defined mesomorphological parameters of the individual CGPs, including the crack length, angle, width, and fracture ratio, present different distribution characteristics in the individual CGPs.

(3) The impact simulations for HCR have been used to examine how the breakage behaviors are affected by the 3D mesostructure under different impact velocities. Both the shape of the gangue phase and approximate location of interfaces are the key parameters that should be taken into account to study the evolution process of mesocracks from bridging into several main fragments. This study demonstrates...
that combining the milli- and micro-XCT tests and image-based DE modelling is an effective technique to investigate the internal damage and failure patterns in HCRs.

**Nomenclature**

\( \rho_c \): The density of the coal phase (kg/m\(^3\))

\( \rho_g \): The density of the gangue phase (kg/m\(^3\))

\( E_c \): The elastic modulus of the coal phase (Pa)

\( E_g \): The elastic modulus of the gangue phase (Pa)

\( \nu_c \): Poisson’s ratio of the coal phase

\( \nu_g \): Poisson’s ratio of the gangue phase

\( R \): The bond radius (m)

\( \sigma \): The friction angle (\(^\circ\))

\( \tau \): Cohesion (Pa)

\( \sigma_{\text{max}} \): The maximum shear stresses (Pa)

\( \tau_{\text{max}} \): The maximum tensile stresses (Pa)

\( \beta_c \): The moment contribution factor

\( K_c/K_g \): Ball stiffness ratio

\( \sigma_t \): Tensile strength, (Pa)

\( \zeta \): Cohesion (Pa)

\( \phi \): Friction angle (\(^\circ\))

\( \beta_n \): Normal damping ratio.

**Data Availability**

The data used to support the findings of this study are available from the corresponding author upon request.

**Conflicts of Interest**

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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