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A Data Mining Method for Constitutive Model of Hard Brittle Coal

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Abstract: - Data mining is an effective way to solve various types of complex nonlinear problems. And the anisotropy of the mechanical characteristics of coal is a typical nonlinear problem. Hard coal seam are usually characterized by brittleness, which makes them difficult to be crushed efficiently. It is important to improve the efficiency of hard coal crushing by the brittleness characterization method of hard coal is clarified. So the constitutive model and damage mechanism of hard brittle coal was studied in this paper. Damage model of hard brittle coal based on Weibull distribution was established. The damage transition point concept was proposed based on the deformation stage characteristics of hard brittle coal. And effective damage intervals for hard brittle coals can be determined based on the damage transition point. Uniaxial compression experiments of hard brittle coal were simulated using EDEM. The characterization of the effect of discrete elemental eigenstructural parameters on the brittleness of coal was analyzed. And quantitative relationships between shear modulus and brittleness, brittleness and damage transition point were fitted by Matlab. A discrete elemental constitutive model for hard brittle coals was obtained. Finally, the correctness of discrete elemental constitutive model was verified by comparing uniaxial compression experiments with other specimens. The results of this paper were expected to provide a theoretical basis for the crushing technology of hard brittle coal. And the numerical theoretical basis for data mining of the intrinsic model of hard and brittle coal was provided.

Keywords: Data Mining (DM), Intelligent Simulation (IS), Hard Brittle Coal (HBC), Discrete Constitutive Model (DCM), Damage Mechanism (DM).

I. INTRODUCTION

Data mining is a hot issue in the field of artificial intelligence and databases. The key data evolution of various complex models can usually be obtained by data mining [1-3]. The anisotropy of coal is a key issue that affects the effectiveness of crushing and support in the field of coal production. Main reason lies in the lack of clarity in the variation of the mechanical characteristics of coal under various operating conditions. And data mining provides a solution to these problems. In the context of the increasing proportion of hard and brittle coal, previous data mining and state prediction methods based on single machine models have been unable to meet crushing requirements due to low efficiency and poor accuracy. By establishing a data mining prediction model for the constitutive characteristics, feature extraction is performed from massive monitoring data. Then, based on the extracted feature data, the property changes are predicted. By introducing the concept of big data, the connections between different data are mined, further enhancing the ability to handle fuzzy data.

At present, complex coal seam geological conditions have a series of engineering problems for mainstream mining technology [4-7], which are characterized by high hardness or high brittleness. These conditions lead to high energy consumption and severe wear and tear of the picks in conventional mechanical cutting technology. The lump rate of mined coal is low and the powder phenomenon is serious [8-10]. Therefore, it is important to clarify the ontological characteristics of hard brittle coal to improve mining efficiency. Li et al. [11] analyzed the stress interference mechanism of highway surrounding rock and carried out similar experiments based on continuous mechanics. Chen et al. [12] believed that the intermediate deformation of the elastic phase will affect the final fracture shape, which is why an elastic fracture model is created based on the specific free energy function and the fracture potential function. Wei et al. [13] studied the dynamic change characteristics of non-destructive rock during fracture and deformation. Oliveira et al. [14] modified the traditional fracture criterion and mechanical model, and studied the relationship between mesoscale rock damage and the instability of the overall bearing capacity.

In most cases, the failure of coal and rock results in sliding of the inner surface of the fracture and generally unstable subsidence, and discontinuous deformation behavior, such as the expansion of rock fractures, can be described by tensile strength theory. Gao et al. [15] and Cao et al. [16] systematically analyzed the hard brittle rock

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mass and explained the failure mode of hard brittle rock over time through the aging safety model of engineering rock mass based on the theoretical time model. Pathiranagei et al. [17] established a statistical coupled TM constitutive model for sandstone based on Weibull distribution and Lemaitre"s strain equivalent principle. Jia et al. [18] and Wang et al. [19] revealed the relationship between stress concentration coefficient and principal stress by analyzing environmental characteristics and roadway fracture patterns, and analyzed the influence of parameters such as rotation Angle on rock mechanics design models. Zhu et al. [20] studied the damage characteristics of brittle rocks, confirmed the irreversible thermodynamic theory, and established a model of irreversible conditions under hydraulic action.

The above theoretical studies have defined the constitutive characteristics and the crushing mechanism of coal and rock breaking means. However, most of the existing achievements are aimed at the traditional conditions of high-quality coal, and there is no coal breaking mechanism applicable to hard brittle coal. For the research background of this paper, that is, hard brittle coal, the existing methods are difficult to apply to the mechanical properties of hard brittle coal, and there is not much in-depth research on the brittle characteristics of coal, so it is necessary to further clarify the physical properties of hard brittle coal, build a constitutive model of hard brittle coal conditions and its crushing mechanism under the synergistic effect of impact and cutting.

In this paper, limitations of existing brittleness indicators were analyzed. Damage modeling of hard brittle coal was proposed. And using the data mining method, the quantitative relationship between the constitutive parameters and the brittleness characteristics of coal was analyzed. Discrete element constitutive model of hard brittle coal was developed.

II. Brittleness Analysis Considering Energy Release of Coal

A. Limitations of Existing Brittleness Indexes

The brittleness of coal refers to the characteristics that when the external force of coal reaches a certain limit, there is only a small deformation and failure, and the carrying capacity is lost. Brittleness is usually measured by brittleness. The greater the brittleness, the more obvious the brittleness of the coal. At present, the slope between the peak strength and the remaining strength during the post-peak decline in the post-peak compressive deformation curve of the commonly used stress-strain curve represents the brittleness of coal and rock, as shown in Figure 1.

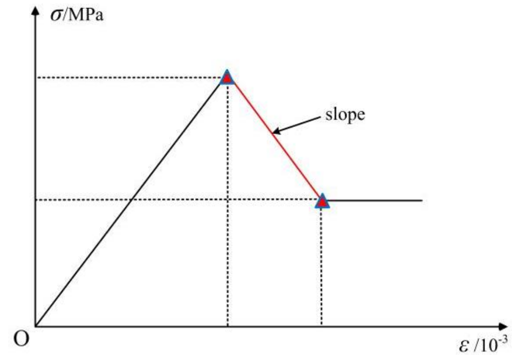


Figure 1: The Brittleness Characterization Method of Coal Rock with the Post-Peak Slope of Compressive Stress-Strain Curve

Due to non-uniform medium of coal, the coal rock has several stress drops, and its pores are accompanied by a small stress drop in the process of compression failure. Since the coal body has not penetrated, the coal still has a certain carrying capacity after the small stress drop. When the pores in the coal are loaded, new cracks appear at the position where they meet the failure criteria, resulting in new stress drops. Due to the high porosity of coal body, the stress-strain line of coal body has a long nonlinear elastic section and a short pre-peak plastic zone, as shown in Figure 2. Traditional brittleness index is difficult to characterize the brittleness of hard coal, so it is necessary to establish a new brittleness index to characterize the brittleness of coal.

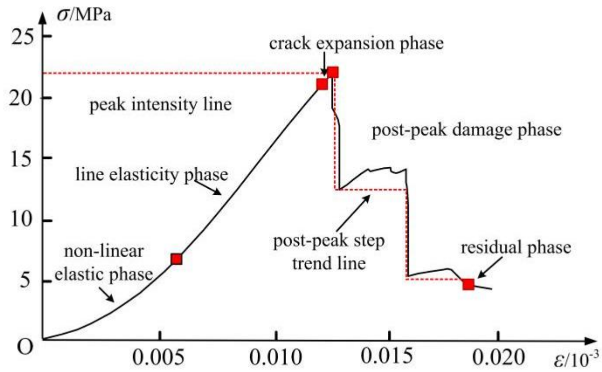


Figure 2: Phased characteristics of stress-strain curve of hard brittle coal

B. Brittleness Analysis Considering Energy Release

Based on the energy dissipation theory, this section analyzes the energy release law of hard brittle coal. And uses the energy release velocity of coal specimen in the post-peak failure stage to characterize the brittleness of coal.

1) Pre-peak Failure Stage: According to the energy change analysis of the stress-strain curve shown in Figure 2, the uniaxial compression process of coal specimen is divided into three stages: non-linear elasticity, linear elasticity and crack propagation, and the energy geometric model of the pre-peak failure stage is obtained, as shown in Figure 3. The U_{df} region represents the plastic effect when the coal body is unloaded before the peak stress. Under ideal circumstances, if the uniaxial compression test is loaded to unload near point A, the energy change in the U_{df} region is the sum of the dissipated energy of the coal body in the pre-peak failure stage, and the energy change in the U_{sf} region is the sum of the internal energy of the coal body in the pre-peak failure stage.

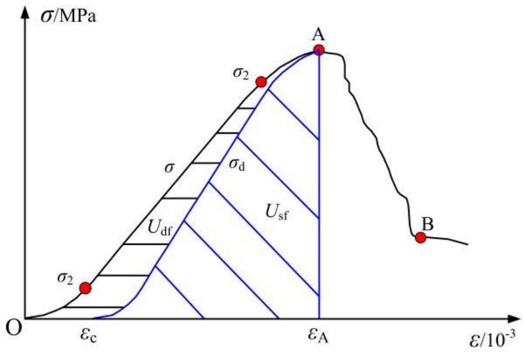


Figure 3: Energy Geometry Model of unloading in Pre-Peak Failure Stage

If a hard brittle coal specimen is taken as a reference, the total work done by mechanical energy W_{mf} is

$$W_{\mathrm{mf}} = V\int_0^{\varepsilon_A} \sigma d\varepsilon \tag{1}$$

Where, V is the volume, mm^3; ε_A is the strain corresponding to the ultimate failure stress of the coal specimen. σ is the stress change curve of the coal specimen at the loading stage, MPa.

The total of pre-peak internal energy changes is

$$\Delta U_{\mathrm{sf}} = V\int_{\varepsilon_c}^{\varepsilon_A} \sigma_{\mathrm{d}} d\varepsilon \tag{2}$$

Where, σ_d is the stress change curve of coal specimen during unloading stage, Mpa; ε_c is the maximum strain after unloading in the pre-peak failure stage.

Finally, the pre-peak dissipative energy increment ΔU_{df} is

$$\Delta U_{\mathrm{df}} = V\int_0^{\varepsilon_A} \sigma d\varepsilon - V\int_{\varepsilon_c}^{\varepsilon_A} \sigma_{\mathrm{d}} d\varepsilon \tag{3}$$

2) Post-peak Failure Stage: As can be seen from Figure 2, in the post-peak failure stage of coal specimens, considering that the post-peak failure stage of coal presents a ladder-like feature, for hard brittle coal, the change of dissipated energy is basically reflected in the process of stress decline, and the change of internal energy is basically reflected in the process of stress stabilization or recovery. The energy change analysis is carried out in combination with the stress-strain curve of the post-peak failure stage, as shown in Figure 4. U_{sp} region represents the plastic effect in the post-peak failure stage, and the energy change in this region is the sum of the internal energy of the coal body in the post-peak failure stage, while the energy change in U_{dp} region is the sum of the dissipated energy of the coal body in the post-peak failure stage.

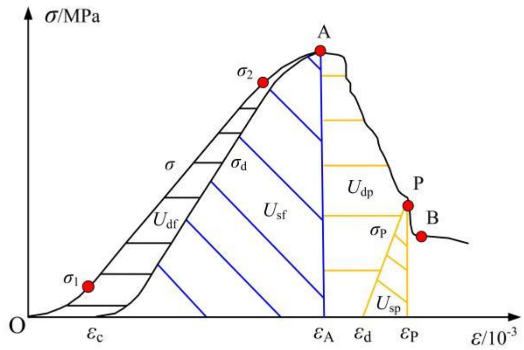


Figure 4: Geometric model of energy unloading in post-peak failure stage

When point P is residual point B, post-peak mechanical energy work W_{mb} is

$$W_{\text{mb}} = V\int_{\varepsilon_A}^{\varepsilon_B} \sigma d\varepsilon \tag{4}$$

Where, ε_B is the strain value corresponding to the residual point.

The post-peak strain energy increment ΔU_{sb} at residual point B is

$$\Delta U_{\text{sb}} = V\int_{\varepsilon_d}^{\varepsilon_B} \sigma_P d\varepsilon - V\int_{\varepsilon_c}^{\varepsilon_A} \sigma_d d\varepsilon \tag{5}$$

The final post-peak dissipative energy increment ΔU_{db} is

$$\Delta U_{\text{db}} = V\int_{\varepsilon_A}^{\varepsilon_B} \sigma d\varepsilon + V\int_{\varepsilon_c}^{\varepsilon_A} \sigma_d d\varepsilon - V\int_{\varepsilon_d}^{\varepsilon_B} \sigma_P d\varepsilon \tag{6}$$

3) Simplification of the Energy Model of Brittleness: It is known from the analysis in the above section that the brittleness of coal is reflected in the energy Angle as the release rate of the accumulated internal energy in the post-peak failure stage. Therefore, if B_r represents the brittleness of coal, then

$$B_r = \frac{\Delta U_{\text{db}}}{W_{\text{mb}}} \tag{7}$$

Where ΔU_{db} is the increment of dissipated energy in the post-peak fall process, J; W_{mb} is the work done by mechanical energy in the post-peak stage, J.

According to (4), (6) and (7), the brittleness can be obtained as

$$B_r = \frac{V\int_{\varepsilon_A}^{\varepsilon_B} \sigma d\varepsilon + V\int_{\varepsilon_C}^{\varepsilon_A} \sigma_d d\varepsilon - V\int_{\varepsilon_d}^{\varepsilon_B} \sigma_p d\varepsilon}{V\int_{\varepsilon_A}^{\varepsilon_B} \sigma d\varepsilon} \tag{8}$$

Considering that the brittleness calculation method represented by (8) is relatively complex, and for hard brittle coal, it is difficult to calculate the plastic strain in its pre-peak failure stage, so (8) is simplified.According to previous studies, the pre-peak energy calculation method for hard rock is $\sigma^2/(2E_{AO})$, while hard coal is different from hard rock in that the proportion of non-linear elastic failure stage is usually large. First, the energy change at this stage is accurately calculated. As can be seen from Figure 4, the pre-peak energy calculation method is $\int_0^{\varepsilon_A} \sigma d\varepsilon$. Secondly, because the proportion of crack growth stage of hard brittle coal is often small, if the unloading is carried out at this stage, the plastic strain generated is also irreversible, but basically negligible. Meanwhile, the change of elastic modulus in the crack growth stage is also related to the degree of crack development in the coal body. It can be obtained as

$$E_B = (1 - D)E_A \tag{9}$$

Where, E_A is the ideal elastic modulus of coal specimen, MPa; E_B is the elastic modulus of crack growth stage, MPa; D is the damage variable. Considering the small proportion of crack growth stage of hard brittle coal, $E_B \approx E_A$ is taken as $D \approx 0$. In order to facilitate calculation, $E_B = E_{AO}$ is taken, where E_{AO} is the secant modulus of peak point, MPa.

In the post-peak failure stage of coal, if the coal is unloaded at point P, the energy change at this time is similar to that of hard rock. Therefore, the internal energy accumulation at point P is simplified as $\sigma_P^2/(2E_{AO})$, and the internal energy accumulation at residual point B is $\sigma_B^2/(2E_{AO})$.

Finally, considering the stepped characteristics of coal in the post-peak failure stage, the comprehensive energy change of this stage should be accurately calculated, that is, $\int_{\varepsilon_A}^{\varepsilon_B} \sigma d\varepsilon$.

Therefore, the brittleness characterization method was finally simplified as

$$B_{\mathrm{r}} = \left(\int_{\varepsilon_{\mathrm{A}}}^{\varepsilon_{\mathrm{B}}} \sigma d\varepsilon - \frac{\sigma_{\mathrm{B}}^{2}}{2\mathrm{E}_{\mathrm{AO}}} \right) \Big/ \int_{\varepsilon_{\mathrm{A}}}^{\varepsilon_{\mathrm{B}}} \sigma d\varepsilon \quad (10)$$

For intuitive representation, the simplified crispness geometric model constructed is shown in Figure 5. The area of the horizontal line represents $\int_{\varepsilon_A}^{\varepsilon_B} \sigma d\varepsilon$, and the area of the tilting dashed triangular line represents $\sigma_B^2/(2E_{AO})$, where E_{AO} is secant modulus.

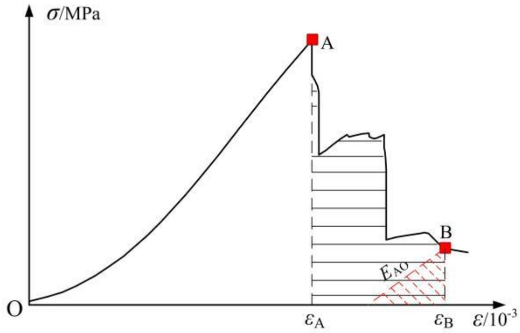


Figure 5: Geometric Model of Brittleness Characterization of Hard Brittle Coal

III. MECHANICAL CHARACTERISTICS ANALYSIS OF HARD BRITTLE COAL BASED ON DAMAGE MODEL

A. *Establishment of Damage Model of Hard Brittle Coal*

According to previous studies, the existing damage variable D constructed based on damage area is

$$D = \frac{A_1}{A_0} = \frac{1 - \overline{A}}{A_0} \quad (11)$$

Where, A_1 is the damage area of the bearing surface, mm^2; $\overline{A}$ is the effective cross-sectional area after damage, mm^2; A_0 is the initial surface area of the bearing surface, mm^2.

If the total number of coal particles is N and the number of destroyed particles under a certain load is N_c, then both exist

$$D = \frac{N_C}{N} \quad (12)$$

The concept of effective stress is

$$\tilde{\sigma} = \frac{S_s}{A_0 - A_1} \quad (13)$$

Where S_s is the axial force of the section, kN.

According to elasticity, the apparent stress σ is satisfied

$$\sigma = \frac{S}{A_0} \quad (14)$$

The combination (11), (13), (14) can be obtained

$$\tilde{\sigma} = \frac{\sigma}{1 - D} \quad (15)$$

According to Hooke's law, there is

$$\varepsilon_i = \frac{(1+\mu)\tilde{\sigma}_i - \mu(\tilde{\sigma}_1 + \tilde{\sigma}_2 + \tilde{\sigma}_3)}{E} \quad (16)$$

Where, ε_i is the main strain, mm; $\overline{\sigma}_i$ is the effective principal stress, i=1,2,3, MPa; E is the elastic modulus, MPa; μ is Poisson's ratio.

By substituting (15) into (16), there is

$$\varepsilon_i = \frac{\sigma_1 - \mu\sigma_2 - \mu\sigma_3}{E(1 - D)} \quad (17)$$

Thus have

$$D = 1 - \frac{\sigma_1 - \mu\sigma_2 - \mu\sigma_3}{E\varepsilon_1} \quad (18)$$

When only the uniaxial stress state is analyzed, σ_1=σ_2=0, then there is

$$D = 1 - \frac{\sigma}{E\varepsilon} \tag{19}$$

The damage elastic modulus is set as $\tilde{E}$, which can be obtained according to the effective stress theory

$$\sigma = \tilde{E}\varepsilon \tag{20}$$

By substituting (19) into (20), there is

$$D = 1 - \frac{\tilde{E}}{E} \tag{21}$$

Let the destruction criterion of the element be

$$s(\sigma) = c_\sigma \tag{22}$$

Where $s(\sigma)$ is some combination function of stress; c_σ is a constant. This formula shows that failure occurs when the stress level $s(\sigma)$ in the element reaches its strength c_σ. In addition, the stress-strain relationship of coal particles before failure obees Hooke's law, so (22) can be rewritten as

$$f(\varepsilon) = c_\varepsilon \tag{23}$$

Let c_ε satisfy some probability distribution, the density function is p, when the strain combination interval is [F, $F+dF$], the probability p_f of microelement failure can be expressed as

$$p_f = p(F)dF \tag{24}$$

Thus, in this region, the microelement dN_c of the entire coal body failure can be expressed as

$$dN_c = N \cdot p_f = N \cdot p(F)dF \tag{25}$$

Under the action of load, when the strain combination of coal body reaches a certain level F, the number of destroyed microelements in the coal body, N_c, is the sum of the damaged microelements in each interval, then

$$N_c = \sum_0^F dN_c = \int_0^F Np(x)dx = NP(F) \tag{26}$$

Where, P represents the distribution function corresponding to the probability density function p.

By substituting (26) into (12) and (18), the damage model of hard brittle coal is finally obtained

$$P(F) = D = 1 - \frac{\sigma_1 - \mu\sigma_2 - \mu\sigma_3}{E\varepsilon_1} \tag{27}$$

B. Constitutive Relationship of Coal Based on Weibull Damage Model

In this section, the constitutive relation of limiting uniaxial compression is taken as an example. the constitutive equation of coal body based on Weibull damage model is obtained

$$\sigma = \exp\left[-\left(\frac{\varepsilon}{\varepsilon_{\mathrm{A}}}\right)^{M_0'}\right]E\varepsilon \tag{28}$$

The stress-strain process of hard brittle coal as shown in Figure 2 is simplified to Figure 6. Stage I is the nonlinear elastic deformation stage. Stage II is the linear elastic deformation stage. Stage III is the crack expansion stage, and stage IV is the failure stage. Among them, stage III is the key for hard brittle coal to break coal, and its high brittleness makes the internal crack propagation stage of coal more short than that of conventional coal. The transition point of this stage is marked as S. At this time, hard brittle coal is basically compacted under external load, and all mechanical parameters are basically close to the homogeneous state, and all parameters become constant.

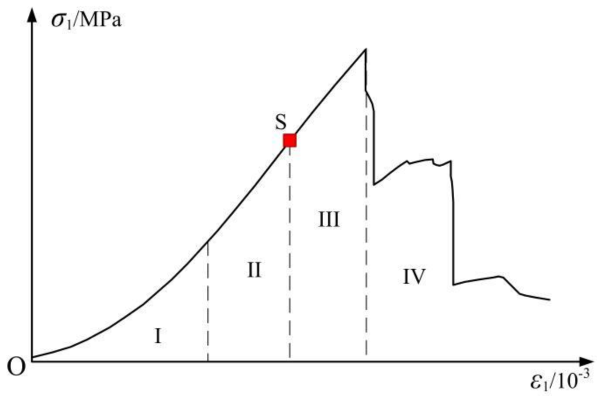


Figure 6: Deformation and Failure Process of Hard Brittle Coal

According to the characteristics of deformation stage of hard brittle coal, the following assumptions are made:

- As a porous medium, coal body has initial damage, denoted as D_0.
- The coal body damage at the transition point S becomes 0, where the strain is denoted as ε_s and the stress is denoted as σ_s.
- The above elastic modulus constant can be used as a partial elastic model without damage, denoted as E.
- It is assumed that starting from the transition point, the coal microelement strength follows Weibull distribution.

Under this condition, the coal damage constitutive model can be divided into two parts, the first part of the strain from 0 to ε_s, damage variable from D_0 to 0. The latter part of the strain goes from ε_s to failure, and the damage variable goes from 0 to 1.

Based on the above hypothesis, the constitutive relation of coal damage considering initial damage is given as

$$\sigma=\begin{cases}\exp\left[-\left(\dfrac{\varepsilon_s-\varepsilon}{\varepsilon_A-\varepsilon_s}\right)^{B_r z}\right]E\varepsilon,\varepsilon<\varepsilon_s\\ \exp\left[-\left(\dfrac{\varepsilon-\varepsilon_s}{\varepsilon_A-\varepsilon_s}\right)^{\frac{z}{B_r}}\right]E\left(\varepsilon-\varepsilon_s\right)+\sigma_s,\varepsilon\geq\varepsilon_s\end{cases}\tag{29}$$

Where, B_r is the brittleness of coal, which is obtained from Equation (10); z is the statistical parameter of Weibull distribution, and its determination method is:

$$z=\frac{1}{\ln\left(E\varepsilon_{\max}/\sigma_{\max}\right)}\tag{30}$$

The coal damage model corresponding to (29) is

$$D=\begin{cases}1-\exp\left[-\left(\dfrac{\varepsilon_s-\varepsilon}{\varepsilon_A-\varepsilon_s}\right)^{B_r z}\right],\varepsilon<\varepsilon_s\\ 1-\exp\left[-\left(\dfrac{\varepsilon-\varepsilon_s}{\varepsilon_A-\varepsilon_s}\right)^{\frac{z}{B_r}}\right],\varepsilon\geq\varepsilon_s\end{cases}\tag{31}$$

To determine the position of the transition point S (ε_s,σ_s), let D=D_0 when ε=0, then

$$1-\exp\left[-\left(\frac{\varepsilon_s}{\varepsilon_A-\varepsilon_s}\right)^{B_r z}\right]=D_0\tag{32}$$

By solving (32), the transverse position of crack propagation transition point of hard brittle coal can be obtained.

IV. Numerical Simulation of Discrete Element Experiment

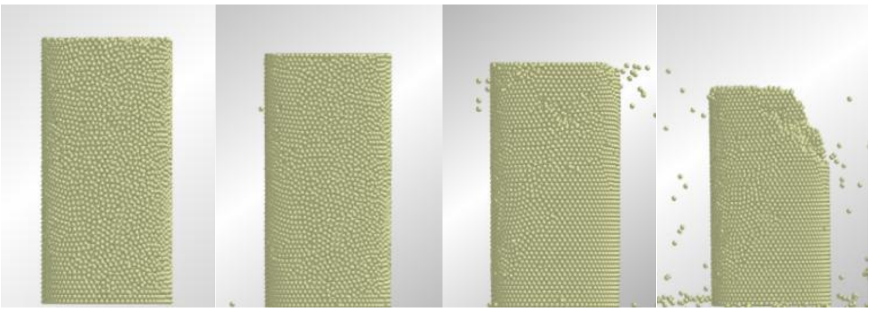
A. *Stress-strain Relationship of Conventional Hard Coal*

In this section, the conventional hard coal model is simulated by using discrete element method, and the stress-strain relationship of the model is obtained by uniaxial compression simulation experiment, and the rationality of the relationship between the brittleness evaluation and the damage constitutive relationship is verified. According to the uniaxial compression test standard, the model size of the coal body is set as 50mm×100mm, the particle unit size and accumulation quantity according to previous research, the filling volume fraction is about 0.61, the particle radius is 1mm, and the accumulation quantity is 28,502. In terms of mechanical parameters, the calculation method for parameter setting of hard coal in EDEM software has been given in current studies. The coal measure selected for coal hardness *f*5 is taken as the research object in this section, and its mechanical parameter setting is shown in Table 1. After the coal specimen model is stacked up and the bonding bond is generated, the lateral constraint of the coal body is removed, and the upper boundary is set to be loaded downward at a speed of 1mm/min. The coal specimen is significantly damaged as the node, and the compression process of the coal specimen is finally obtained, as shown in Figure 7.

Table 1: Mechanical Parameter Setting of Coal Specimen Model

Hardness	f5
Poisson's Ratio	0.17
Shear Modulus(GPa)	1.620
Density(kg/m3)	1420
Coefficient of Restitution	0.45
Coefficient of Static Friction	0.48
Coefficient of Rolling Friction	0.18
Normal Stiffness per unit area(GN/m3)	1900
Shear Stiffness per unit area(GN/m3)	810
Critical Normal Stress(MPa)	50
Critical Shear Stress(MPa)	20
Bonded Disk Radius(mm)	1

In Figure 7, (a) is the original model of the coal specimen. In order to facilitate the description, the compression process is divided into three stages: (b)-(d). Figure (b) is the compaction stage. Figure (c) shows the fracture failure stage. It can be seen that the particle arrangement on the surface of the coal specimen has been disordered, and some particles have fallen off at the top of the specimen, indicating that permanent damage has occurred inside the specimen at this time. Figure (d) is the stage of peel failure, it can be seen that a large coal body has separated from the specimen, and it is manifested as shear failure.



(a) (b) (c) (d)

Figure 7: Uniaxial Compression Process of Coal Specimen

From the perspective of the overall process of uniaxial compression of coal specimens, the physical law shown is consistent with the actual situation, and the simulation results can be used for analysis in subsequent studies. Therefore, the EDEM post-processing module calculates the pressure on the upper boundary during the compression of coal specimens, and takes this as the stress data of coal specimens, and converts the time point of the compression process into the displacement of the upper boundary. The ratio of 100mm to the height of the specimen is taken as the strain data of the coal specimen, and the stress-strain relationship is thus obtained, as shown in Figure 8.

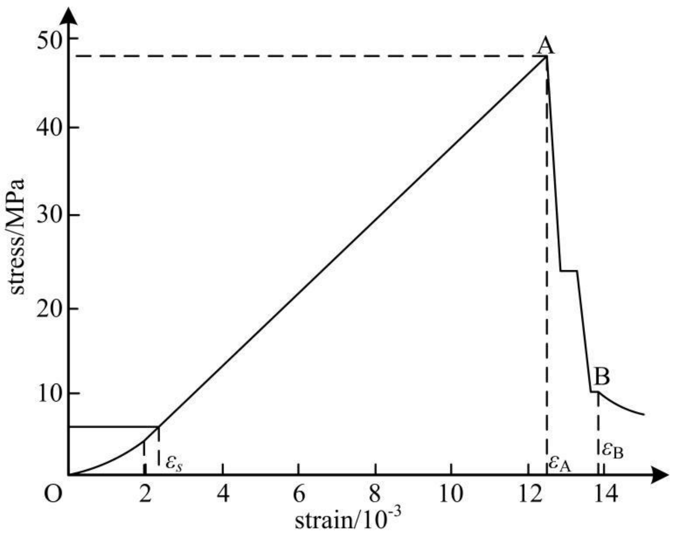


Figure 8: Stress-strain relationship of conventional hard coal specimen with hardness of *f*5

As can be seen from Figure 8, the peak stress of the coal specimen in the compression process is about 48MPa, which is relatively close to the ultimate compressive strength of 50MPa when the coal hardness is *f*5, according to the empirical conversion formula of the ultimate compressive strength and the Platts coefficient of coal hardness. In terms of brittleness value, according to (10), the obtained stress-strain data are imported into Matlab to obtain the integral value of $\varepsilon_A \to \varepsilon_B$. Since the corresponding value of σ_B is known, E_{AO} takes secancy modulus, that is, the ratio of σ_A to ε_A, and finally obtains brittleness B_r of about 0.5783, that is, quasi-brittle coal. As for the damage transition point, it can be seen from (30) and (32) that the initial damage D_0 should be required for the calculation of the damage transition point. Since there is a nonlinear elastic deformation stage in Figure 8, and the transverse coordinate corresponding to the turning point is about 2, it can be regarded as about 0.2% of the coal specimen model with damage, so the initial damage D_0 is 0.002. The damage transition point ε_s is about 2.3120, and the corresponding damage transition stress σ_s is about 6.0839MPa.

In conclusion, the uniaxial compression simulation experiment of conventional hard coal specimen with hardness *f*5 is consistent with the actual law, which can be used as the basis and comparison content for the subsequent research on the influence of discrete constitutive parameters on the brittleness of coal. At the same time, the calculation of brittleness value and damage transition point in the simulation results shows that the brittleness characterization and damage constitutive relationship have a good echo effect, and the rationality is verified, which can be used as a theoretical basis for subsequent research.

B. Analysis of the Influence of Discrete Element Constitutive Parameters on the Brittleness of Coal

In EDEM software, the parameters related to the mechanical properties of materials are Poisson's ratio, shear modulus, unit method/tangential stiffness and critical method/tangential stress respectively. The definition objects of Poisson's ratio and shear modulus are particle elements, and the definition objects of unit/tangential stiffness and critical/tangential stress are adhesive bonds. Considering that the macroscopic mechanical properties of the coal model built depend on adhesive bonds, and the mechanical concept of Poisson's ratio is not assigned to adhesive bonds, this parameter is excluded first. The critical method/tangential stress reflects the hardness of coal, which is calculated by the Prevois coefficient of coal hardness. If the value is changed, its hardness will also change, which is obviously not suitable for analysis. The unit method/tangential stiffness is derived from the shear modulus calculation, which is the key to unify the mechanical characteristics of the particle element and the bond. It can be understood as the deformation resistance of the bond. The smaller the stiffness, the easier it is to deform, and the larger the stiffness, the harder it is to deform. Therefore, this section will take shear modulus as a variable to study its influence on the brittleness of coal.

In the selection of the range of variables, it is considered that the strain ε_A corresponding to the stress peak σ_A in the uniaxial compression experiment has the following relationship with the elastic modulus E:

$$\sigma_A = E\varepsilon_A \tag{33}$$

As the ideal value of σ_A in the study in this section is constant at 50MPa, the theoretical strain εA value of each simulation scheme is distinguished to facilitate the comparative analysis of the simulation results. Therefore, the elastic modulus of the reference coal measure of the hard coal specimen in Section 4.1 is 3.80GPa. According to the relation $E=G\cdot 2(1+\mu)$ between elastic modulus E and shear modulus G and Poisson's ratio μ, and the conversion relation between shear modulus and bond stiffness, the values of shear modulus of each simulation scheme are set as shown in Table 2.

Table 2: Shear Modulus and Bond Stiffness of Each Scheme

Scheme	1	2	3	4	5
Shear Modulus(GPa)	1425	1526	1943	2137	2374
Normal Stiffness per unit area(GN/m^3)	1667	1785	2273	2711	2777
Shear Stiffness per unit area(GN/m^3)	712	763	971	1068	1187

The setting of other parameters is the same as that in Table 1, and the upper boundary is also set to be loaded at a speed of 1mm/min. The stress-strain relationship of coal specimens of each scheme is finally obtained, as shown in Figure 9.

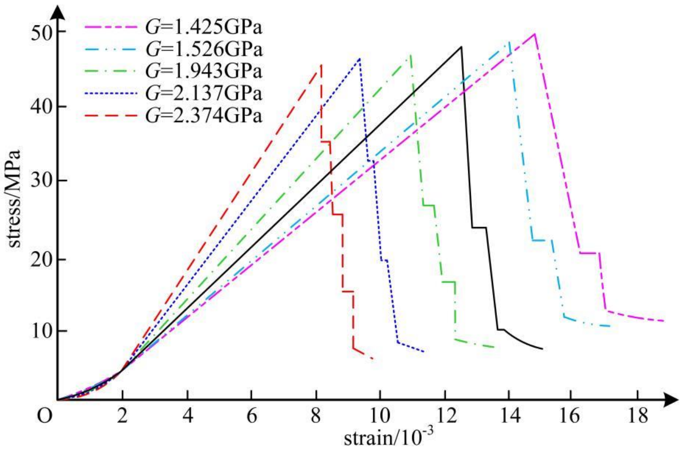


Figure 9: Stress-strain Relationship of Coal Specimens under Each Scheme

As can be seen in Figure 9, with the increase of shear modulus and bonding bond stiffness, the peak stress and residual strength of coal specimens become smaller, but the critical normal stress of bonding bond under each simulation scheme is set at 50MPa. Theoretically, the peak stress of coal models with different stiffness should maintain a high uniformity even if it does not reach 50MPa. The reason for this phenomenon may be that the increase of stiffness makes the energy transferred by the bonding bond when it generates unit displacement larger, which leads to a wider range of damage in the coal body, and the coal body strength deteriorates more. As the strain continues to increase, the coal body strength decreases continuously. When the strain reaches the critical value, the peak strength and residual strength of the specimen are lower than the theoretical value. At the same time, this explanation can also reasonably explain that the strain corresponding to the stress peak decreases with the increase of the shear modulus and the stiffness of the bonding bond, that is, the increase of the stiffness of the coal body increases the energy transferred when the bonding bond produces unit displacement, and the total boundary displacement required for the coal body to produce macroscopic crushing decreases, which is then reflected in the decrease of the strain variable at the stress peak. On the other hand, in the post-peak failure stage of coal specimens, with the increase of shear modulus and bond stiffness, the step-like feature of stress-strain curve becomes more obvious, and the decline rate is faster. The reason may be that the energy required for bond displacement increases due to the increase in stiffness, and constant energy storage is needed to realize bond displacement before deformation. This phenomenon can be understood as the increase of stiffness reduces the propagation efficiency of energy inside the coal body, which is ultimately reflected in the reduction of the scope of single macroscopic damage of the coal body and the increase of the number of times required to achieve complete damage, that is, the ladder-like feature.

In order to analyze the brittleness characteristics of coal specimens with different shear modulus and the change characteristics of damage transition points, the brittleness values and damage transition points of each scheme were obtained according to the calculation method of the compression simulation results of coal specimens in Section IV. A, as shown in Table 3.

Table 3: Brittleness Value and Damage Transition Point of Each Scheme

Scheme	1	2	Original	3	4	5
Brittleness B_r	0.5319	0.5507	0.5783	0.7427	0.7981	0.8425
Damage Transition Strain ε_s(10^{-3})	0.9981	1.0422	2.3120	5.3775	6.5803	6.9149
Damage Transition Stress σ_s/MPa	1.8243	1.8026	6.0839	21.4794	31.1885	38.2608

By analyzing the data from Table 3 and Figure 9, it can be seen that the strain value at the peak compressive stress of coal specimens of all schemes basically changes uniformly with the change of shear modulus, and there is little difference between the brittleness value of serial number 1 and 2 and the damage transition strain and the damage transition stress. However, since the setting of the shear modulus of the original specimen, the three indexes of the specimen have improved significantly. Compared with the original specimen, the three indexes of serial number 3 showed a rapid increase. Starting from the setting of shear modulus of serial number 4, the rising rate of the three indexes gradually flattens out. From this phenomenon, the following conclusions can be drawn: In terms of brittleness value, the increase of shear modulus and stiffness can improve the brittleness of coal, and there is a certain parameter critical point, when the shear modulus exceeds the point, the brittleness value will increase significantly; In terms of damage transition point, the increase of shear modulus and stiffness will delay the location of the transition point, and there is a certain parameter critical point, when the shear modulus exceeds the point, the damage transition point will be delayed to a large extent.

In order to obtain the quantitative relationship between the shear modulus and the brittleness of coal, the data in Table 3 are imported into Matlab for fitting. Considering that the main research object of this paper is hard brittle coal, the skew-plastic coal with too small brittleness value is not considered for the time being. Therefore, according to the variation range of the simulation results, the variation range of the shear modulus is preset as 1GPa-3GPa. According to the principle that the brittleness value should not exceed the interval (0,1), each fitting type is screened, and the fitting curve of brittleness value B_r and shear modulus G is obtained, as shown in Figure 10.

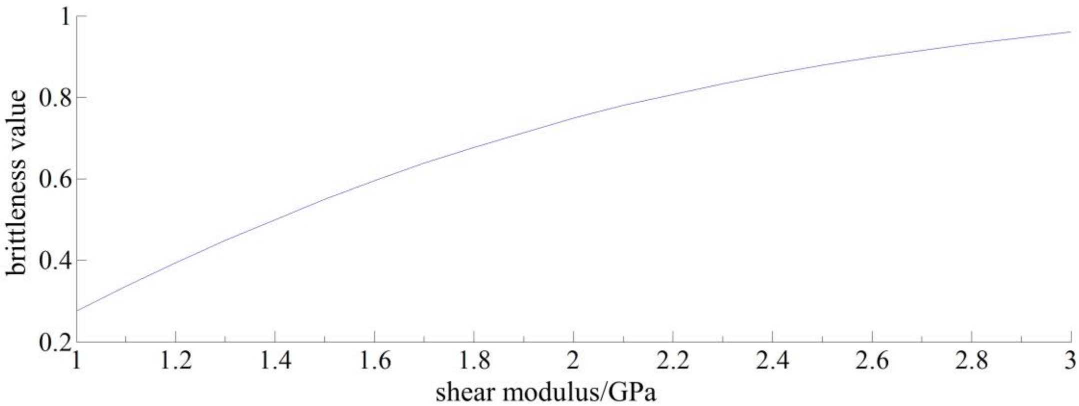


Figure 10: Fitting Curve of Shear Modulus G and Brittleness Value B_r

The corresponding fitting relationship in Figure10 is

$$B_r = -0.2477\sin(G-\pi) - 0.02677(G-10)^2 + 2.236 \tag{34}$$

The quantitative relationship between brittleness and damage transition point is further analyzed. Due to the change of shear modulus, the stress peak and strain value will change. If the data in Table 3 are directly fitted, the stress and strain value corresponding to the damage transition point may exceed the stress peak and strain value, which is obviously inconsistent with the actual situation. Therefore, the fixed position of the damage transition point is converted to the relative position based on the peak, and the quantitative relationship between it and the shear modulus is analyzed. According to the transverse and longitudinal coordinates corresponding to the peak value of each simulation scheme in Figure 9, the ratio of damage transition strain to stress relative to the peak value was calculated, as shown in Table 4. The data were imported into Matlab for fitting, and the fitting types were screened according to the principle that the relative proportion of damage should not exceed the interval (0,1). The fitting curve between the relative position of the damage transition point and the brittleness value is shown in Figure 11.

Table 4: Relative Positions of Damage Transition Points and Peak Values in Each Scheme

Scheme	1	2	Original	3	4	5
Strain of Peak ε_A(10^{-3})	14.8247	14.0185	11.5118	10.9216	9.3381	8.0813
Relative Proportion of Damage Transition Strain(%)	6.7327	7.4345	20.0837	49.2373	70.4672	85.5667
Stress of Peak σ_A(MPa)	49.6341	48.3573	47.8736	46.6820	46.4659	45.6410
Relative Proportion of Damage Transition Stress(%)	3.6755	3.7277	12.7083	46.0122	67.1213	83.8299

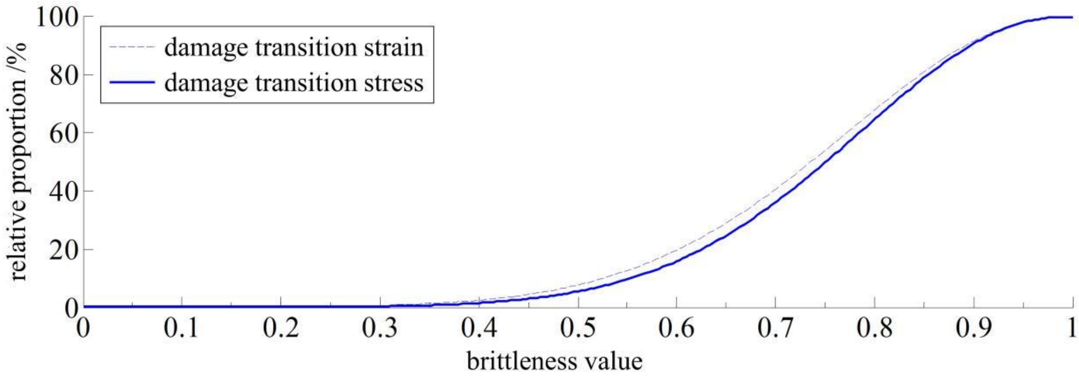


Figure 11: Fitting curve of relative position of damage transition point and brittleness value B_r

Let η_ε represent the relative proportion of damage transition strain and η_σ represent the relative proportion of damage transition stress. The fitting relationship corresponding to Figure 11 is as follows:

$$\left.\begin{aligned} \eta_\varepsilon &= 99.45e^{-\left(\frac{B_r-0.9895}{0.3055}\right)^2} \\ \eta_\sigma &= 99.47e^{-\left(\frac{B_r-0.9884}{0.2862}\right)^2} \end{aligned}\right\} \tag{35}$$

In summary, Equations (34) and (35) are discrete element constitutive models of hard brittle coal with hardness of *f*5.

C. Verification of Discrete Element Constitutive Model of Coal with Different Hardness

Considering that the stress limit strength of coal with different hardness is different, the strain value at the stress peak is also different. Therefore, the accuracy of the discrete element constitutive model established in Section IV. B needs to be verified under different hardness conditions. Coal specimens with hardness *f*4 and *f*6 are taken as the research object. As for the setting range of shear modulus, it can be seen from (10) that the brittleness value is obtained by the integral of the stress-strain curve in the post-peak stage, that is, it is related to the area in the post-peak stage. Therefore, the shear modulus of conventional coal specimens with different hardness corresponding to Table 1 can be calculated as:

$$G = G_{f5} \times \left(\frac{f}{5}\right)^2 \tag{36}$$

Where, G_{f5} is the shear modulus and GPa of the original specimen under the hardness of *f*5.

According to (36), when calculating the brittleness value of coal with different hardness, its shear modulus should be similar to the shear modulus under *f*5 hardness. and then according to (34), the theoretical brittleness value of coal specimens with different hardness under this shear modulus can be obtained as follows:

$$B_r = -0.2477\sin\left(\frac{25}{f^2}G - \pi\right) - 0.02677\left(\frac{5}{f}G - 10\right)^2 + 2.236 \tag{37}$$

By comparing the simulation results with those calculated in (37), the accuracy of the discrete element constitutive model can be verified. It is now known that the shear modulus of the original specimen is 1.620GPa. According to (36), the shear modulus of the conventional coal specimen with *f*4 and *f*6 hardness is 1.037GPa and 2.333GPa respectively. According to the method described in Section IV. B, the other two shear modulus values are set respectively under each hardness for uniaxial compression simulation experiment. The specific parameters are shown in Table 5. And the stress-strain relationship of coal specimens under each scheme is shown in Figure 12.

Table 5: Mechanical Parameters of f4 and f6 Hardness Coal Specimens

Scheme	1	2	3	4	5	6
Hardness	*f*4	*f*4	*f*4	*f*6	*f*6	*f*6
Shear Modulus(GPa)	1.006	1.037	1.075	2.231	2.333	2.444
Normal Stiffness per unit area(GN/m^3)	1177	1213	1258	2610	2730	2859
Shear Stiffness per unit area(GN/m^3)	503	519	538	1116	1167	1222
Critical Normal Stress(MPa)	40	40	40	60	60	60
Critical Shear Stress(MPa)	16	16	16	24	24	24

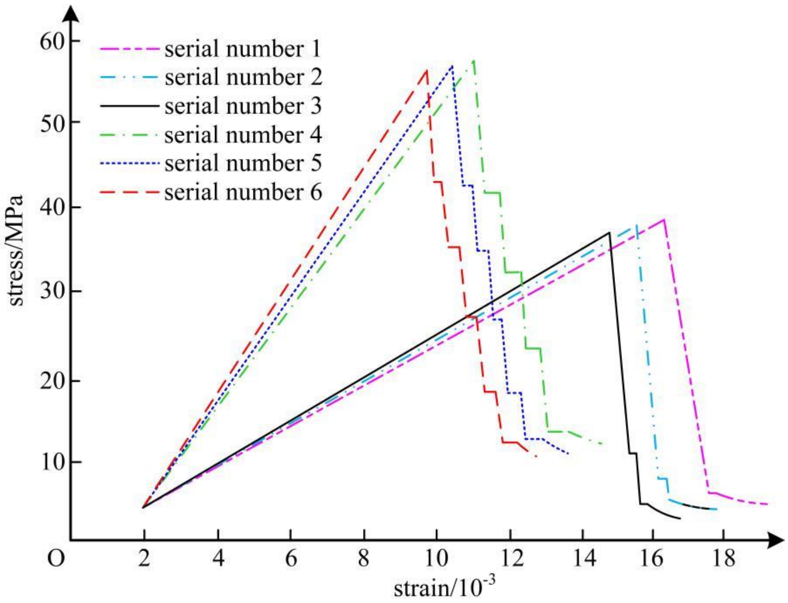


Figure 12: Stress-strain Relationship of *f*4 and *f*6 Hardness Coal Specimens

As can be seen from Figure 12, with the increase of hardness of coal specimens, the peak stress of coal specimens in the compression process is higher and higher, and they are all close to the theoretical value, and the strain decreases with the increase of hardness of specimens, which is consistent with the actual law. The data are further imported into Matlab, and the simulated and theoretical values of brittleness under each scheme are calculated respectively, as shown in Table 6.

Table 6: Simulated and Theoretical Values of Brittleness of *f*4 and *f*6 under Each Scheme

Scheme	1	2	3	4	5	6
Simulated Brittleness Value	0.4283	0.4501	0.4858	0.7024	0.7685	0.7763
Theoretical Brittleness Value	0.4376	0.4554	0.4763	0.7095	0.7461	0.7841

The embrittlement value obtained by simulation is close to the theoretical embrittlement value, and the error is less than 3%, indicating that the embrittlement calculation method of (37) is correct.

As for the damage transition point, the ratio of strain to stress at the peak value was also calculated according to the simulated damage transition results, and then the theoretical value of the relative proportion of damage transition was calculated according to (35), as shown in Table 7.

Table 7: Simulated and Theoretical Values of the Relative Proportion of Damage Transition of f4 and f6 under Each Scheme

Scheme	1	2	3	4	5	6
Simulated Damage Transition Strain(10^{-3})	0.6159	0.7052	0.8533	4.7429	5.4297	6.2810
Simulated Strain Relative Proportion(%)	3.7659	4.5389	5.8013	43.0617	52.1865	63.9156
Theoretical Strain Relative Proportion/%	3.8040	4.6794	5.9162	42.9324	52.7140	63.2828
Simulated Damage Transition Stress(MPa)	0.9338	1.1338	1.4719	22.3478	27.3147	33.9195
Simulated Stress Relative Proportion(%)	2.4254	3.0075	3.9781	38.8657	48.0892	60.3550
Theoretical Stress Relative Proportion(%)	2.4499	3.1005	4.0480	38.4831	48.5749	59.7574

It can be seen that the relative proportion of damage transition obtained by simulation is relatively close to the theoretical value, and the error is less than 2%, indicating that the brittleness calculation method of (35) is correct.

To sum up, the discrete element constitutive model about brittleness and damage transition point of coal body is correct, and for coal body with different hardness, calculation should be combined with (37).

V. CONCLUSIONS

In this paper, based on the limitations of existing coal brittleness characterization, the brittleness index of coal was proposed. The constitutive relationship of hard brittle coal based on damage mechanics was defined. And the discrete elemental constitutive model was established based on data mining method. The main conclusions are as follows:

- According to the step-drop stress-strain curve of coal, the limitations of the existing brittleness indexes were pointed out. The energy evolution laws of the pre-peak and post-peak stress stages of coal under loading conditions are analyzed. And the brittleness characterization method of hard brittle coal was defined.
- The uniaxial compression test of conventional coal specimens was simulated by using EDEM discrete element method. The discrete element constitutive model of hard brittle coal was obtained. And the correctness of

discrete elemental constitutive model was verified by comparing uniaxial compression experiments with other specimens.

- The damage transition point proposed in this paper helps to find an effective crushing method for hard brittle coal by calculating the optimal damage interval of coal, thus improving the crushing efficiency of hard brittle coal.

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