The research macro-mechanical properties of rock based on discrete particle model

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Abstract. The influences of different microscopic parameters of the macroscopic mechanical properties are not the same. Based on discrete element granular flow theory, particle contact stiffness, friction coefficient, connection strength and other microscopic parameters of the material properties of macroscopic mechanical properties are analyzed combined with laboratory experiments. Using triaxial test to study Ⅳ surrounding rock specimen under different mechanical properties. Based on discrete element granular flow theory, using PFC2D to analyze the relationship between different microscopic parameters and macroscopic mechanical properties. It is found that particle contact stiffness has great influence on the peak strength, macroscopic initial tangent modulus and elastic modulus; With the increase of the friction coefficient between the particles, the peak strength increases; connection strength is greater, the greater the material cohesion and Poisson's ratio is smaller. Research results may reflect the influences of microscopic parameters on the macroscopic mechanical properties of materials, and provide a basis for the selection of microscopic parameters in the numerical calculation.

1. Introduction

At present, domestic and foreign scholars have proposed many methods to simulate the mechanical properties of the material under external force based on different research purposes and requirements. Generally, the proposed methods are: continuous medium and discrete element. According to the function of discrete element method, it can be divided into macroscopic and microscopic discrete elements. The former focuses on solving problems (UDEC and 3DEC) caused by relatively large discontinuities (such as faults, joints and joints surface between structure and foundation, etc.); while the latter is mainly used for discontinuous contact surfaces or points (PFC, YADE) with large number, for example, the contact surfaces and points between the rupture surfaces of rock mass, or between the particles of the materials. A famous scholar, Peter Cundall, by using the theory of microscopic discrete elements, developed the discrete element numerical PFC commercial software [1-2], which is widely applied to solve various problems of research material microstructure.

A foreign scholar, Bagnold, was the first one to reveal the constitutive relation between the particles. In the 1950s, Bagnold conducted a coaxial shear rheological test for wax ball by using glycerin - alcohol - aqueous solution, and then proposed the famous Bagnold's law [3]. Then Ogawa introduced the concept of "granular temperature", and on this basis, the kinetic theory of granular flow model was rapidly established. The study on particle flow began to develop quickly after 1970s. In 1979, Cundall and Strack first developed a two-dimensional discrete element simulation program for

studying the mechanical properties of particulate media, which were the beginning of discrete element simulation of particle motion [4-6].

At present, the discrete element PFC program referring to the field of rock engineering is mainly applied to the fracture brittle and mechanical properties simulation of hard rock mass, strength characteristics of jointed rock mass and rock engineering [7-9]. M. Doležalová et al. [10] studied the effect of stress path on the basic characteristics of the material by using PFC; for PFC applications, the Japanese scholars have been in a leading position, of which T. Hoda and I. Towhata have successfully solved the liquefaction and stability problems of the dam under seismic loading by using PFC[11]. Xu Jinming et al.[12] taking an example of limestone, obtained the mechanics data of rock through laboratory experiments, and linked the micromechanics and macroscopic parameters of the particles by using particle flow numerical method, then built a microstructure model of limestone. Based on the particle flow theory, J. W. Park and J. J. Song carried out a 3D simulation [13] for joint direct shear tests with PFC3D software through characterizing joint unit by weakening the strength of the particles. Zhu Huanchun [8] introduced the basic research ideas and work steps of PFC, the model building, the development of rock rupture during the test, changes and failure mode of the stress - strain during the engineering. Nevertheless, there is still no clear explanation for the microscopic parameter selected by the scholars, therefore, there has been a problem referring to the calculation of PFC.

Select the appropriate meso-mechanical parameters of particles is vital for macroscopic stress-strain curves of material simulation. The meso-mechanical parameters of different materials have different effects on the macroscopic mechanical properties. Currently, the tunnel rock mass conditions are not good; the study of the rock material with low strength is few. In this paper, taking an example of grade Ⅳ railway tunnel rock mass, we will analyze the effect of micromechanical parameters of particles, such as contact stiffness, friction coefficient and connection strength on the macroscopic mechanical properties of the material, combining with laboratory tests.

2. Laboratory Test

2.1. Specimen Preparation

Taking a certain grade Ⅳ railway tunnel rock mass for the study, and according to the " Railway Tunnel Design Specifications", the physical parameters of rock mass are as shown in Table 1. Preparation of model material has a similar relation with the values in the table. Materials are mainly composed of sand, fly ash, barite powder, lubricants and water. After conducting a series of trial ratio, that river sand and barite powder are aggregate, and fly ash and lubricants are cement materials can be determined, with the ratio of 1: 1: 0.32: 0.09. Formulation was conducted based on the material mixture ratio, and compacted in a mold by using a compaction meter to achieve the required density, as shown in Fig.1. Model samples are cylindrical, with a diameter of 39.5mm, and a height of 80mm, as shown in Fig. 2.

Table 1 Physico-mechanical indices of grade Ⅳ railway tunnel rock mass

Rock mass grade	Gravity γ (KN/m^3)	The elastic resistance coefficient K (MPa/m)	Deformation modulus E(GPa)	Poisson's ratio μ	Internal friction angle φ (°)	Cohesion c (MPa)	Calculated friction angle φ_c (°)
Ⅳ	20~23	200~500	1.3~6	0.3~0.35	27~39	0.2~0.7	50~60

Table 2 Physico-mechanical properties of samples

No.	Gravity(KN/m^3)	Elastic modulus (MPa)	Poisson's ratio	Flying shears		Triaxial		Rock mass grade
				c (kPa)	φ (°)	c (kPa)	φ (°)	
Model material	21.5	27.8	0.33	14.6	34.9	11.3	Model material	21.5

The untrained triaxial shear was applied to the experiment, with a strain rate of 1%. Through a series of experiments, the physical and mechanical parameters of the complete samples made by this material are shown in Table 2, and the apparatus used in the experiment are shown in Fig. 3.

Fig. 1 Compaction meter and molds

Fig.2 Specimen

Fig.3 Schemes of displacement sensor

2.2. Test Results

For each series of samples, the test was repeated exactly under the same experimental conditions. Three samples were made for each series, and intermediate values were selected as representative test results.
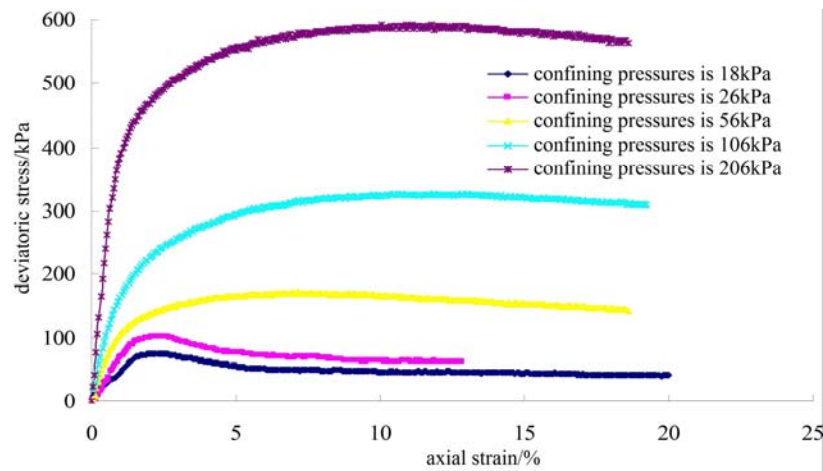
Fig.4 Stress - strain curve with different confining pressures

Under different confining pressures, the grade Ⅳ stress - strain curve of the rock specimen are shown in Fig.4, which shows that: with the increase of confining pressure, peak strength and residual strength increases; the larger the confining pressure, the more obvious the plasticity of the specimen; under low confining pressure (confining pressure of 18,26 KPa), the strength of the specimen increased to its peak and then the stress intensity ddeclined, representing as stress softening, which is the ideal model of elastic-brittle; under high confining pressure, the stress after peak represented as stress hardening, which is the ideal elastoplastic model. The stress - strain curves during cyclic loading and unloading are shown in Fig. 5, of which the fitting curve functions is $\sigma_1 = 27.824\varepsilon_1 - 0.0475$.
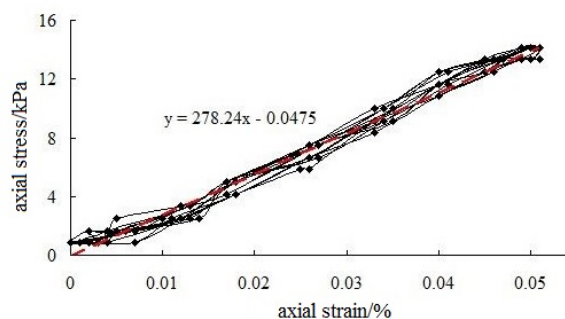

Fig.5 Stress - strain curves during cyclic loading and unloading

3. Research on macroscopic mechanical properties of materials

PFC2D calculation program uses micromechanics mechanics parameters to represent the particles of materials as well as the mechanical properties of their bonding. Before calculating the value of the model, we must first assume several microscopic parameters for the model, and compare the macroscopic mechanical properties and the results obtained in the laboratory. If the result is inappropriate, we need to adjust the parameters of micromechanics, until the calculated results are almost the same as the experimental one, then these parameters can be applied to the actual model calculations. Therefore, the adjustment of microscopic mechanics parameters is very important [14].

3.1. The establishment of specimen model

The sample size is the same as that of during the triaxial experiment of model material, which is 8.0 cm * 3.95cm, the radius of the particles is uniformly distributed within the range of 0.35mm ~ 0.8mm, and the particle density is 2200 kg / m^3. A sample contains a total of 3260 particles, and the sample

parameters are shown in Table 3. For PFC2D, there are two kinds of connection models of particle: contact connection and parallel connection. During the destruction of material particles, the reduction of the stiffness can be modeled by a parallel connection model. As the parallel connection model is more suited for the simulation of rock materials, and it can reflect the cumulative process of material damage, the paper uses a parallel connection model. There are generally three steps for the experimental simulation: generating a sample, consolidation and loading. (as shown in Fig. 6).

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

Fig. 6 The particle flow processes of indoor samples

Table 3 Input parameters of PFC model

Density (kg/m3)	Sample size(cm)	Particle size(mm)	Original porosity	Coefficient of amplification	Normal contact stiffness(GPa)	Stiffness ratio	Friction coefficient	Connection stiffness(kPa)
2200	8.0×3.95	0.35~0.8	0.12	1.6	0.8~40	0.5~8.0	0.1~0.9	0.5~100

By using numerical servo system, PFC maintains a constant confining pressure [14] by the way of adding the loading through relative movement of the top and bottom of the wall while adjusting the displacement on both sides of the wall. Particle distribution after loading the model sample is shown in Fig.6 (d). Throughout the loading and unloading process, PFC program can automatically record the horizontal and vertical stress(σ_x, σ_y)and strain(ε_x, ε_y); wherein, σ_x and σ_y represent the contact area (the side area and top area of the particle sample) divided by the total contact force of the wall and particle.

3.2. Effects of different contact stiffness on macroscopic mechanical properties of materials
Under the conditions that particle friction coefficient of 0.5, the connection strength of 500Pa, with different contact stiffness (8e8, 2e9, 4e9, 8e9 and 4e10), and the calculated stress - strain curve of the model is shown in Fig. 7; and the relationship curve of particle contact stiffness and elastic modulus are shown in Fig.8. As shown in Fig. 7, with the increasing particle contact stiffness, the peak strength of the material also increased, as well as the macro initial tangent modulus, while the axial strain decreases when the shear is being damaged, this has a great influence on the stress - strain curve shape. As shown in Fig.8, the elastic modulus of the material increases along with the increase of the stiffness of particles, this demonstrates a substantial proportional relation.
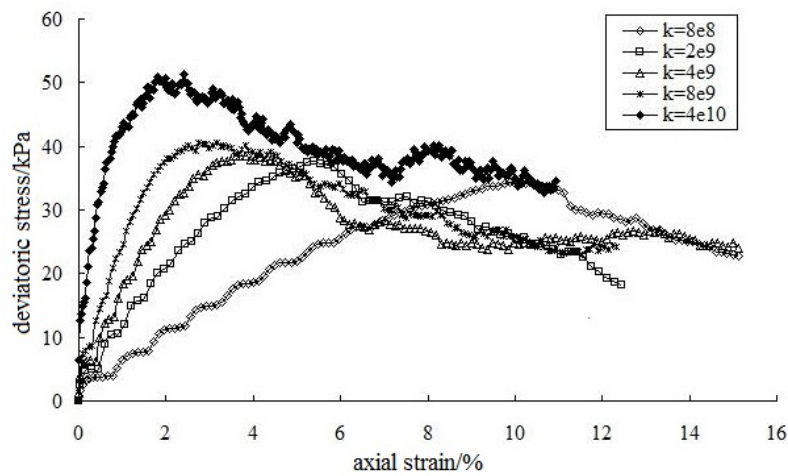
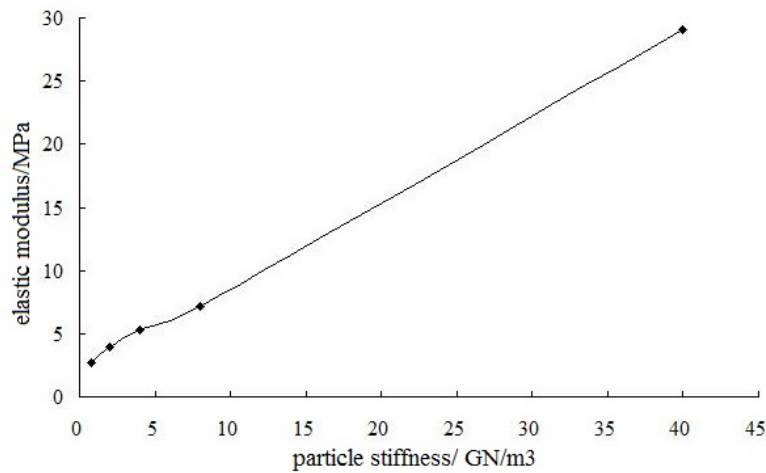**Fig.7** Stress - strain curve with different contact stiffness

Fig. 8 The relationship of particle contact stiffness and elastic modulus

3.3. Effects of different stiffness ratio on macroscopic mechanical properties of materials
Under the conditions of different stiffness ratio (normal stiffness / shear stiffness), respectively 0.5,1,2,4 and 8, the deviatoric stress - strain curves of samples are shown in Fig.9. As can be seen, the stiffness ratio of the material has little effect on the stress - strain curve shape of the material, with little change of the peak strength and residual strength. The relation diagram of stiffness ratio and elastic modulus is shown in Fig. 10. As can be seen from the figure, with the increase of the stiffness ratio, elastic modulus decreases.
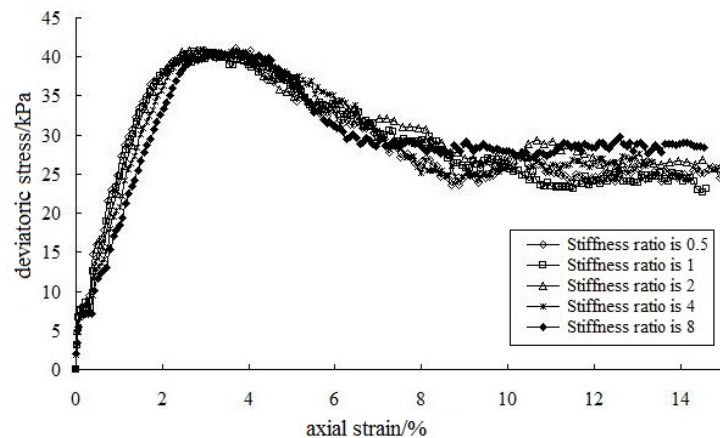
Fig. 9 The stress - strain curve with different stiffness ratio
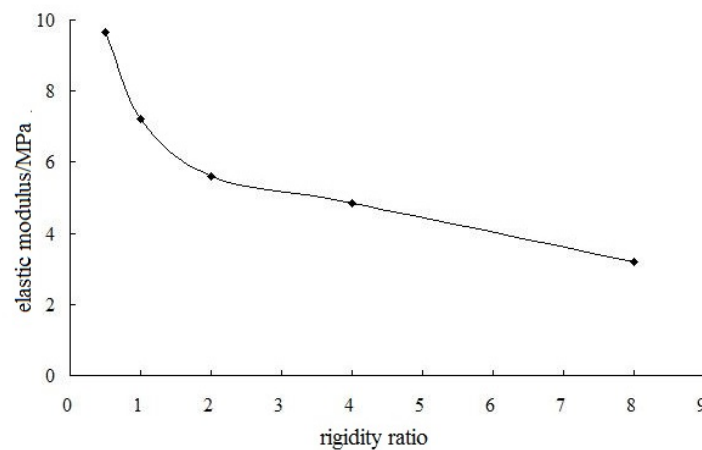

Fig.10 The relationship curve of elastic modulus and rigidity ratio

3.4. Effects of different friction coefficients on macroscopic mechanical properties of materials
Under certain conditions, when the friction coefficient changed from 0.1, 0.3, 0.5, 0.7 to 0.9, the relationship curves between deviatoric stress and axial strain of the sample are shown in Fig. 11, and the relationship curve of peak stress and the friction coefficient are shown in Fig. 12.
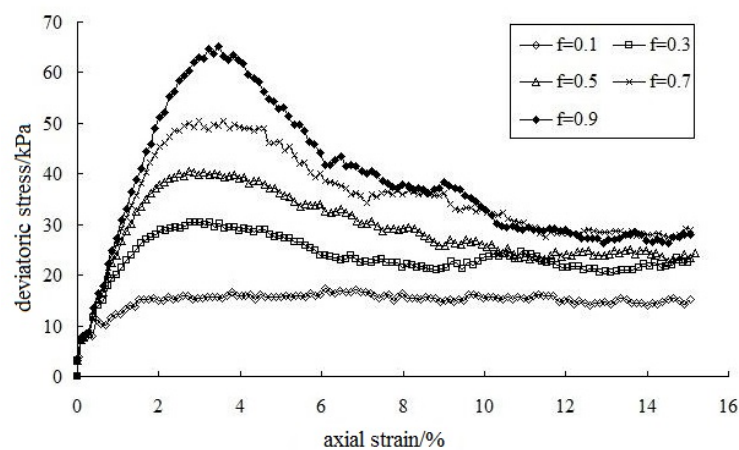

Figure 11 Deviatoric stress - strain curve with different friction coefficients
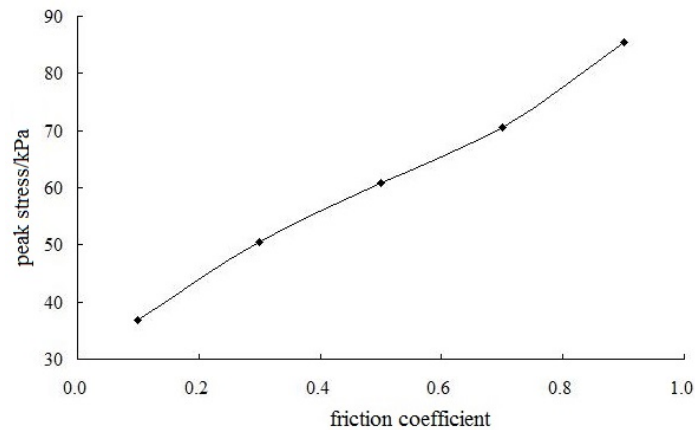
Fig. 12 The relationship curve of peak stress and the friction coefficient

As can be seen in Fig. 11 and 12, that: the peak strength of the sample increases with the increase of the friction coefficient between the particles, substantially representing a direct proportion relationship; when the friction coefficient is small, the material exhibits strain hardening characteristics. The larger the friction coefficient, the material will exhibit strain softening characteristics; residual strength of the material also increases as the friction coefficient increases, but the change is small. In addition, as can be seen in Fig. 11, the variation of friction coefficient has little effect on the initial tangent modulus of the material; this is because of the connection strength between the material particles. Only overcome the connection strength first, can the particles slide. Under the condition of small strain, the connection strength of the model can reach a maximum value; as the strain continues to increase, the model will soon get damaged; after the strain reached a certain value, the volume of the sample would stop increasing; when the stress-strain curve tends to level, only friction component provides strength.

3.5. Effects of different connection strength on macroscopic mechanical properties of materials
Under certain conditions, when the connection strength was taken 0.5 MPa, 5 MPa, 20 MPa, 50 MPa and 100 MPa respectively, the relationship curves of deviatoric stress - axial strain of the samples are shown in Fig. 13. Under different connection strengths, the relationship curves of volumetric strain - axial strain of the materials are shown in Fig. 14. Under different connection strengths, the relationship curves of the connection strength and Poisson's ratio are shown in Fig. 15. The relationship curves of the connection strength and cohesion are shown in Fig. 16.
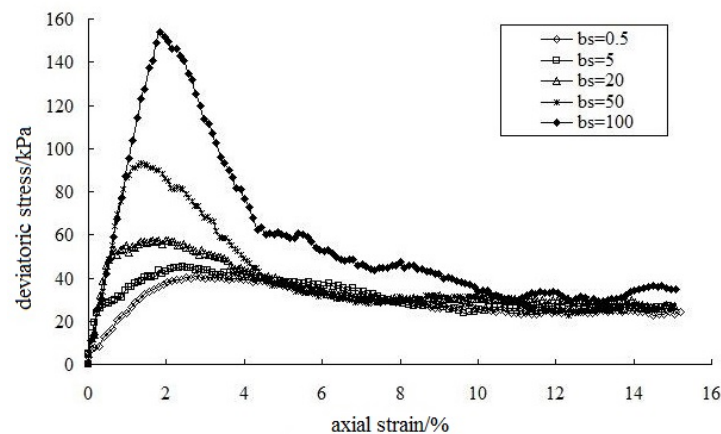

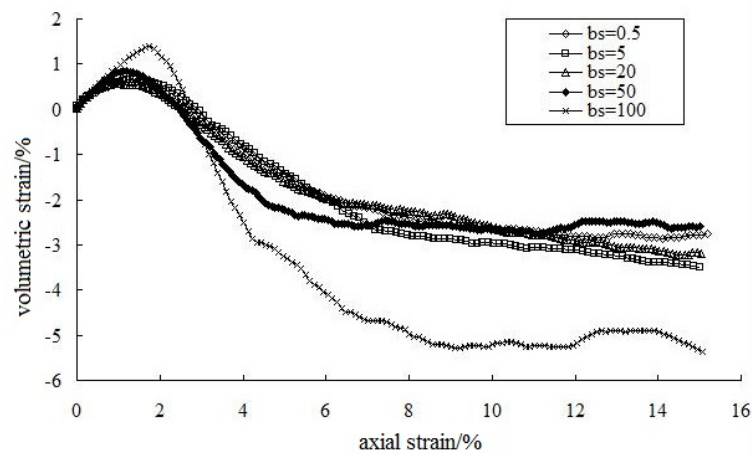**Fig. 13** Deviatoric stress - strain curve with different connection strength

Fig. 14 Volumetric strain - axial strain curve with different connection strength
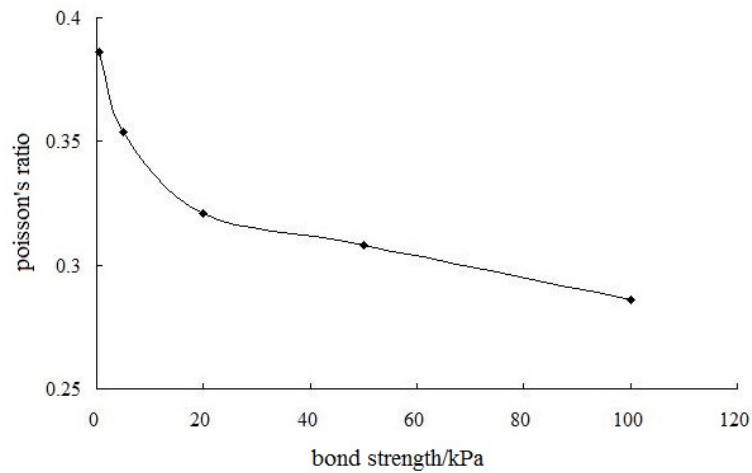

Fig. 15 Connecting the relationship between strength and Poisson's ratio
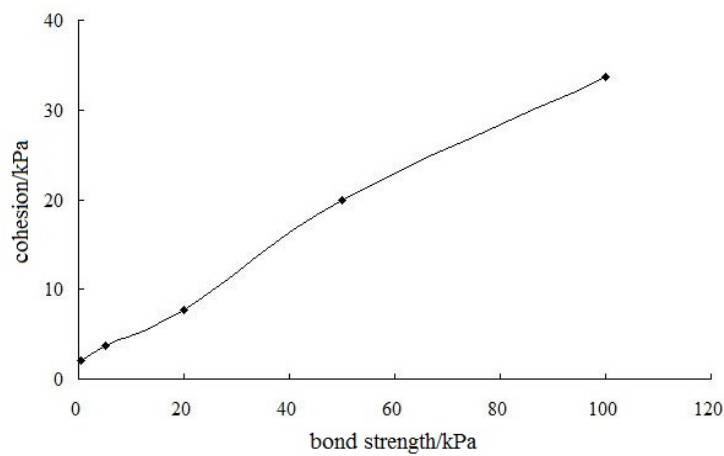

Fig. 16 The curve of Connection strength and cohesion

As it can be seen in Fig. 13 and 16, the greater the connection strength of particles, the greater the peak intensity of the sample; the greater the cohesion of the material, the smaller the Poisson's ratio,

and more obvious the softening characteristics of the stress - strain curve will be. Under different connection strengths, there are little changes in the residual strength of the sample.

In summary, the rule of the influence of each micromechanics parameters of materials on the macroscopic mechanical properties can be obtained. According to the given material stress-strain curves, the microscopic parameters in the PFC calculation model can be adjusted, so as to match the stress-strain curves in the model test. After several adjustments, final parameters and results in the calculation model can be obtained, as shown in Table 4. Fig. 17 is a comparison chart of the test results and calculated results when the confining pressure of the sample is 10KPa.

Table 4 The basic parameters and calculated results of PFC model

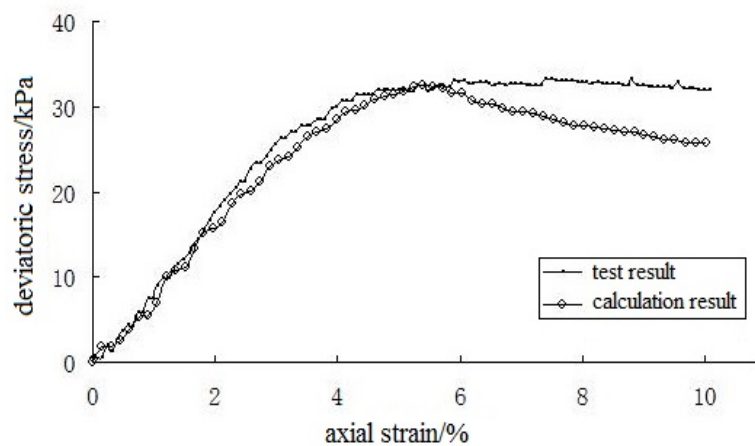| Density (kg/m^3)	Particle size(mm)	Original porosity	Normal contact stiffness(GPa)	Stiffness ratio	Friction coefficient	Connection strength(kPa)	Calculated results			
							E (MPa)	μ	c (kPa)	φ (°)
2200	0.35~0.8	0.16	20	1	0.8	10	26.4	0.35	9.87	32.6

Fig. 17 Stress-strain curve of tests and PFC model

4. Conclusion

Taking the grade Ⅳ railway tunnel rock mass as an example, based on the discrete particle flow theory, combined with the results of laboratory and numerical calculation, we studied the effects of various microscopic parameters of particles including the contact stiffness, the friction coefficient, connection strength on the macroscopic mechanical properties of the materials. The following conclusions can be obtained:

(1) The entire physical mechanical parameters of the specimen similar to grade Ⅳ railway tunnel rock mass can be obtained through a series of laboratory tests.

(2) According to the calculated results, we found that the connection stiffness of particles has a great effect on the stress - strain curve of materials. As the connection stiffness of particles increases, the peak strength of the material increases, as well as the elastic modulus and the macro initial tangent modulus, while the axial strain decreases when the shear failed. And the effect of stiffness on the strain - stress of the material is little.

(3) The peak intensity of the sample will increase proportional with the increase of friction coefficients, and the effect of the friction coefficient on the initial tangent modulus of the material is little, mainly due to the connection strength between the particles of the materials.

(4) With the increase of the connection strength, both the peak strength and cohesion of the sample will increase, Poisson's ratio will decrease, and the more obvious softening characteristic the stress - strain curves of the sample will be. By adjusting the microscopic parameters in PFC calculations, it can well match the test results.

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