

Article

Effect of Confining Pressure on the Macro- and Microscopic Mechanisms of Diorite under Triaxial Unloading Conditions

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Abstract: In this study, the response mechanism between macro- and microscales of deep hard-rock diorite is investigated under loading and unloading conditions. Moreover, the statistical theory is combined with particle flow code simulations to establish a correlation between unloading rates observed in laboratory experiments and numerical simulations. Subsequent numerical tests under varying confining pressures are conducted to examine the macroscopic mechanical properties and the evolution of particle velocity, displacement, contact force chain failures, and microcracks in both axial and radial directions of the numerical rock samples during the loading and unloading phases. The findings indicate that the confining pressure strength curve displays an instantaneous fluctuation response during unloading, which intensifies with higher initial confining pressures. This suggests that rock sample damage progresses in multiple stages of expansion and penetration. The study also reveals that with increased initial confining pressure, there is a decrease in particle velocity along the unloading direction and an increase in particle displacement and the number of contact force chain failures, indicating more severe radial expansion of the rock sample. Furthermore, microcracks predominantly accumulate near the unloading surface, and their total number escalates with rising confining pressure, suggesting that higher confining pressures promote the development and expansion of internal microcracks.

Keywords: deep hard rock; loading and unloading conditions; microscopic structural response; macrodeformation



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1. Introduction

Underground engineering excavation is a complex process involving loading and unloading, which often leads to engineering disasters such as large deformation of surrounding rock, rock bursts, and rock block peeling [1,2]. Research on the mechanical characteristics and fracture mechanism of surrounding rock under complex unloading stress paths has received widespread attention in the engineering field, prompting a considerable amount of foundational research [3,4]. Traditionally, research has been conducted predominantly at the macro scale, with less in-depth investigation into the microscopic structural damage of rock [5]. Therefore, it is essential to enhance the study of the micromechanical characteristics of rock during unloading to better understand the damage and fracture mechanisms of deep surrounding rock.

Many microscale factors affect the macroscopic mechanical properties of rocks. Lakirouhani et al. [6,7] conducted uniaxial compression and Brazilian splitting tests on rocks, and they found that the macroscopic strength and Young's modulus of rocks exhibit a positive correlation with their grain size and a negative correlation with their quartz mineral content. With advancements in nondestructive testing technology, it has become feasible to study rock damage evolution from a microscopic structural perspective [8]. To more intuitively explore the damage behavior of rock samples, new nondestructive

testing technologies such as X-ray CT scanning [9,10], digital image correlation (DIC) [11], and acoustic emission (AE) [12] have been introduced into rock micromechanical tests in recent years. Researchers such as Raynaud et al. [13], Wang [14], and Chen et al. [15] have utilized CT scanning technology to investigate the three-dimensional (3D) failure morphology of rock samples under different stress paths. However, these studies have not seamlessly integrated CT scanning with the loading environment. In this context, several researchers have investigated the use of real-time CT scanning technology [16,17] in rock mechanics testing. Notably, Glatz et al. [18], Wang et al. [19], and Li et al. [20] employed real-time CT scanning to examine the evolution of damage in various microscopic rock structures. To understand the microcrack evolution characteristics of loaded rocks, Si et al. [21], Peng et al. [22], and An et al. [23] analyzed data from AE detection systems, such as AE events, ringing counts, amplitudes, and spectral distributions, during the rock fracture process under different unloading paths, revealing the microcrack evolution in rocks. Qin et al. [24] and Liu et al. [25] used AE 3D spatial positioning information to reconstruct the crack evolution process in rocks and established a microscopic damage characterization equation for rocks. Moreover, some scholars have utilized a combination of CT scanning, AE, and DIC technologies to investigate the microscopic damage evolution of rocks [26,27]. Although these new, nondestructive testing technologies have played a remarkable role in exploring the microstructural damage of rocks, they are not without limitations. AE signals can be considerably affected by external environmental interference, reducing the accuracy of the crack distribution information obtained. CT scanning tests are costly, and DIC technology is limited to exploring the surface mechanical information of unloaded rock.

With the advancement of computer technology, numerical simulations for exploring the microstructural damage evolution in rocks have become increasingly prevalent. These simulations offer several advantages over traditional experimental tests, including lower costs and the ability to replicate complex conditions that are challenging to achieve in laboratory settings. Consequently, an increasing number of researchers are employing numerical simulations to study the crack evolution process in rocks and to investigate the underlying mechanisms of rock damage and fracture [28,29]. The particle flow code (PFC) based on the discrete element method has emerged as a remarkable tool for examining the fracturing mechanisms of rocks under unloading conditions from a microscopic viewpoint [30,31]. Researchers such as Li et al. [32], Xiong et al. [33], and Yin et al. [34] have utilized PFC^{2D} to investigate the macroscopic mechanical behavior, crack propagation, and evolution of various energy indicators in unloaded rocks, highlighting the impact of unloading rates on microscopic structural damage and fracturing. Furthermore, studies conducted by Zhang [35], Zheng et al. [36], and Uxia et al. [37] using PFC^{3D} have explored the initiation, propagation, connectivity, and spatial distribution of microcracks in rocks during unloading, revealing that the unloading effect contributes to post-peak damage and failure in rocks. To address some of PFC's limitations in simulating rock damage processes, new contact models have been developed [38,39], enhancing the application of PFC to numerical simulations of rock unloading.

Despite extensive research on the micromechanical behavior of unloaded rocks and numerous innovative findings, the investigation into the response mechanism between macro- and microscales during rock unloading remains limited. This study aims to bridge this gap by first validating the microscopic parameters of the numerical model based on laboratory data and subsequently developing custom programming in PFC^{3D} to address the quantitative control of unloading rates in simulations. Subsequent numerical tests on diorite under various confining pressures were conducted to examine the macroscopic mechanical characteristics, particle velocity and displacement, contact force chain failure numbers, and the evolution of crack spatial distribution. Moreover, this study aims to elucidate the macroscopic and microscopic response mechanisms of rock samples during the loading and unloading process.

2. Numerical Tests

2.1. Establishment of the Rock Samples

Indoor triaxial tests were conducted using the SAS-2000 triaxial testing instrument at Xi'an University of Science and Technology. The rock samples, derived from diorite located at a depth of 1600 m in the Qinling Mountains, Shaanxi Province, were used in the experimental tests. The dimensions of the rock samples for the compression and splitting tests were $\Phi 50 \text{ mm} \times H 100 \text{ mm}$ and $\Phi 50 \text{ mm} \times H 50 \text{ mm}$, respectively. These dimensions were replicated for the rock samples to maintain consistency with the indoor experimental tests. To balance the computational cost and accuracy, the particle size within the numerical model was set between 0.6 and 1.5 mm based on existing research [40]. The numerical model, comprising 33,675 rigid particles of varying sizes, is depicted in Figure 1.

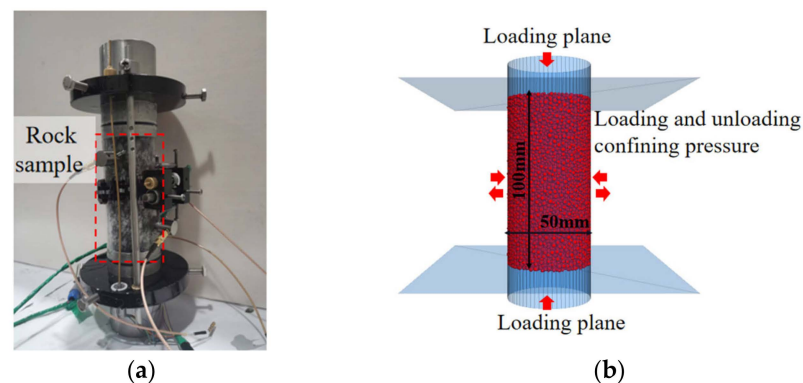


Figure 1. Rock model. (a) Physical experiment model. (b) Numerical model.

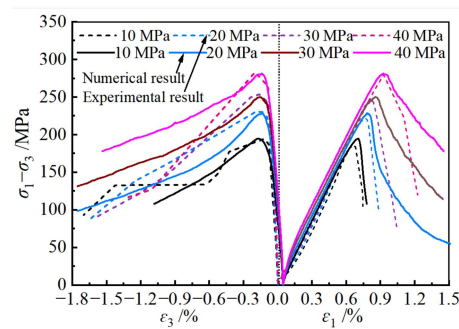
2.2. Determination of Microscopic Parameters and the Unloading Method

In PFC^{3D}, the macro- and microscopic failure phenomena of various rocks are simulated by assigning specific parameters and contact models to the rigid particles and the bonding materials between them. Although several contact models are available, the parallel bond model (PBM) is commonly used for simulating rock materials. However, this model lacks adequate self-locking effects [31]. The flat joint model (FJM) enhances the self-locking effect between particles and addresses the limitations of the PBM, thus proving to be more suitable for simulating the macro- and microscopic mechanical behaviors of rocks [41].

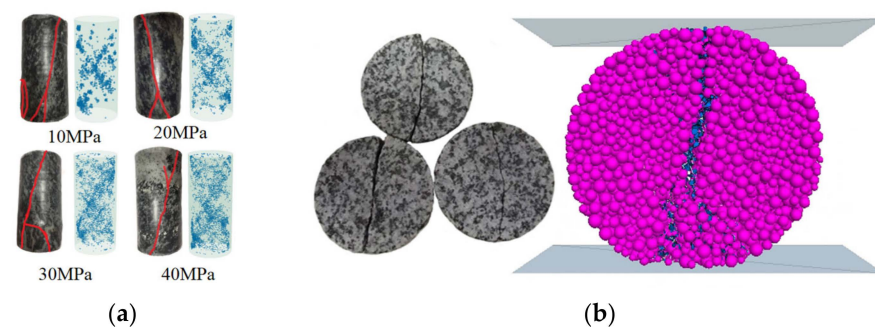
To accurately reflect the macroscopic deformation characteristics of diorite, microscopic parameters within the numerical rock samples were iteratively adjusted using the FJM. To improve calibration efficiency during microscopic parameter verification, the first step is to set the Young's modulus and stiffness ratio of particles and parallel bonds in the numerical model to equal values. Subsequently, the Young's modulus obtained from physical experiments is assigned to the numerical model and continuously adjusted. The Poisson's ratio is verified by changing the stiffness ratio. Next, the matching of tensile and compressive strength between numerical and physical models is achieved by adjusting the parallel bond strength and cohesion. Finally, the particle friction coefficient is adjusted to match the post-peak curves of the numerical and physical models. The optimal set of microscopic parameters that accurately represent the macroscopic mechanical characteristics of diorite is presented in Table 1. Figure 2 illustrates the strength curves obtained from both numerical and indoor experimental tests under various confining pressures.

Table 1. Key microscopic parameters of the FJM.

Microparameter	Value	Microparameter	Value
Particle radius ratio	2.5	Friction coefficient	0.001
Minimum radius/mm	0.6	Internal friction angle/°	4.5
Installation gap/mm	0.2	Elastic modulus/GPa	8.563
Density/kg·m ^{−3}	2710	Bonded tensile strength/MPa	20.02 ± 0.275
Stiffness ratio	2.68	Cohesion/MPa	36.126 ± 1.04

**Figure 2.** Stress–strain curves obtained through experimental and numerical tests.

As can be observed in Figure 2, before attaining the peak strength of the rock samples, the stress–strain curves obtained through numerical and indoor experimental tests display good consistency, and the maximum relative error of peak strength under different confining pressures of 1.83%. Despite some discrepancies after the peak strength, the overall trends are consistent. Figure 3 confirms the similarity in failure modes between the numerical and indoor experimental tests, validating the chosen set of microscopic parameters for subsequent numerical testing.

**Figure 3.** Failure results obtained through experimental and numerical tests. (a) Triaxial compression failure mode. (b) Splitting test failure mode.

The unloading method for confining pressure adopted in this study involves stress reduction per time step without moving the specimen sidewalls, as this approach helps prevent the occurrence of error phenomena, namely confining pressure decreasing and then subsequently increasing during the unloading of confining pressure. The stress/time step unloading method utilizes a servo program to incrementally decrease the predetermined stress at each time step, which can either follow a linear or a nonlinear trajectory. Figure 4 illustrates the unloading strength curves of rock samples derived from both indoor experimental and numerical tests under a confining pressure of 30 MPa. The indoor experimental tests were conducted at an unloading rate of 0.008 MPa/s, whereas the numerical tests employed an unloading rate of 0.002 MPa/step. The similarity in the slope of the unloading strength curves during the unloading process in both tests indicates the efficacy of the stress/time step unloading method in replicating the effects observed in indoor experimental tests (Figure 4).

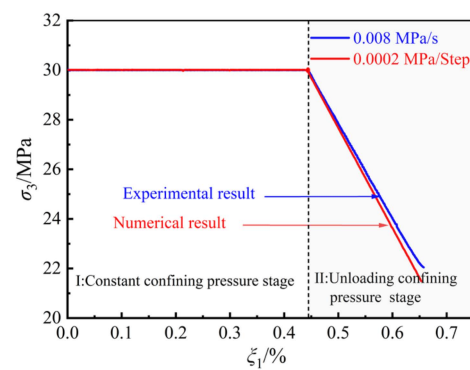


Figure 4. Unloading strength curves obtained through indoor experimental and numerical tests.

2.3. Numerical Test Procedures

To assess the impact of confining pressure on the microstructure of diorite during the unloading process, the following numerical test procedures were implemented:

(1) Utilizing the servo control program in PFC, axial and confining pressures were simultaneously applied to the specimen. Upon reaching the predetermined confining pressures (10, 20, 30, and 40 MPa), the confining pressure was maintained to be constant, and the axial pressure was incrementally applied to the top and bottom surfaces of the rock samples using a displacement control method (0.0002 mm/step).

(2) When the axial stress of the sample achieved 80% of its peak strength, the confining pressure was gradually reduced at a rate of 0.00004 MPa/step while maintaining the axial loading rate constant until the sample failed.

2.4. Division of Axial and Radial Ranges of the Rock Sample

The primary macroscopic deformation directions in a loaded rock sample are axial and radial. To investigate the influence of confining pressure on the internal microstructural response during the macroscopic deformation of the rock sample, the spatial region of the sample was segmented, as shown in Figure 5. In this segmentation, A_i and R_i ($i = 1, 2, 3, 4$, and 5) denote the specific axial and radial ranges within the rock sample, respectively. The macroscopic deformation of the loaded sample reflects the collective behavior of its internal microscopic particles, contact force chains, and microcrack evolution. Microscopic response data from four critical points—A (the initial point of unloading confining pressure), B (90% of peak strength), C (peak strength), and D (60% of peak strength)—on the loading and unloading strength curves under various confining pressures (10, 20, 30, and 40 MPa) were analyzed, as shown in Figure 6.

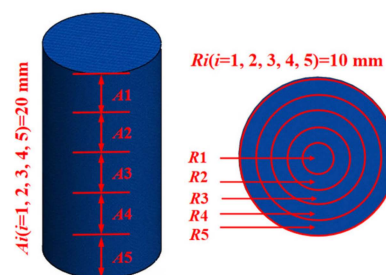


Figure 5. Segmentation of the numerical model into different regions.

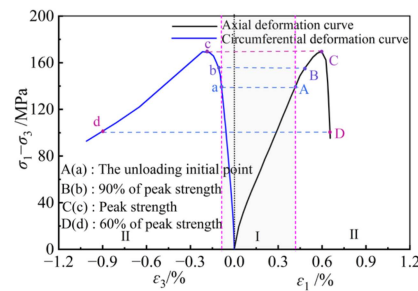


Figure 6. Diagram illustrating key points on the strength curves during loading and unloading.

3. Numerical Results

3.1. Loading and Unloading Strength Curves

Following the numerical test procedures outlined in Section 2.3, numerical tests on the loading and unloading of diorite were conducted. Figure 7 presents the loading and unloading strength curves of diorite under varying confining pressures.

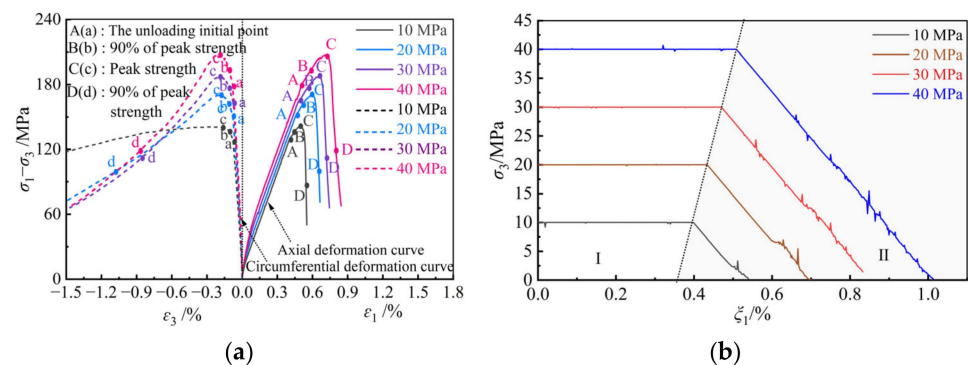


Figure 7. Loading and unloading strength curves of diorite under different confining pressures. (a) Stress–strain curves. (b) Relation between confining pressure and axial strain.

As depicted in Figure 7a, the strength curves of the rock samples exhibit distinct differences under various confining pressures. With an identical unloading rate, the peak deviatoric stress of the rock samples increases with confining pressure, indicating an enhancement in the maximum load-bearing capacity of the samples. This observation aligns with findings from existing research [42,43], suggesting that higher confining pressures enhance lateral constraints on the rock samples, thereby facilitating more effective stress transfer and adjustment among internal particles.

Figure 7b illustrates that during the loading phase (I), the confining pressure remains relatively constant, displaying a horizontal trend as axial strain increases. In the initial stage of unloading (II), the confining pressure decreases linearly with axial strain. As unloading progresses, instantaneous fluctuations in local confining pressure become evident, particularly at higher confining pressures. This behavior indicates that the damage and fracture of the rock samples under loading and unloading conditions transition from sudden to gradual failure, progressively escalating from localized fractures to comprehensive failure.

3.2. Contact Force Chain Response Characteristics

Under external loads, the internal particles of the numerical sample form a complex force chain structure to withstand these loads. The number of failed contact force chains reflects the extent of damage and fracture in the rock sample during the loading and unloading process. Figure 8 displays the variation in the number of failed contact force chains in different axial and radial regions throughout the loading and unloading process of rock samples under various confining pressures.

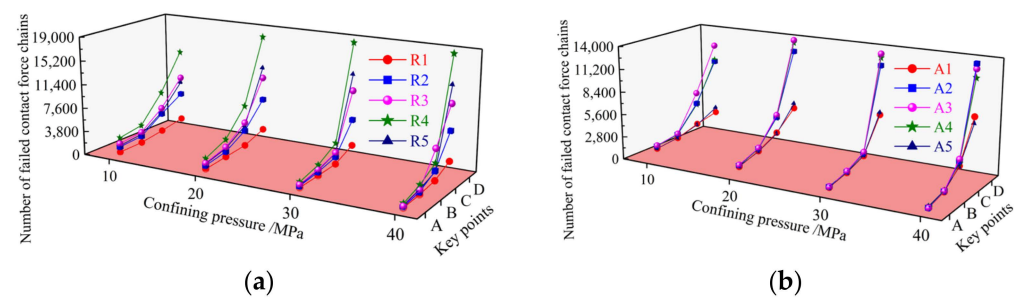


Figure 8. Trends in the number of failed contact force chains in axial and radial directions. (a) Axial direction of the rock sample. (b) Radial direction of the rock sample.

Figure 8a,b show the changes in the number of failed contact force chains along the axial and radial directions of the rock sample, respectively. In the initial unloading phase (A to B), the number of failures is relatively low but increases considerably during the B-to-C and C-to-D stages. Before reaching peak strength, the failure number under low confining pressure exceeds that under high confining pressure. However, after reaching peak strength, the trend reverses, with higher failure numbers observed at higher confining pressures. This pattern indicates that internal damage and fractures in the rock samples decrease before the peak and increase after the peak as the confining pressure increases.

The trend of contact force chain failures during loading and unloading of the rock samples under different confining pressures is nonlinear and concave upward (Figure 8). Beyond the peak strength (C to D), the number of failed contact force chains within the A1 and A5 ranges along the axial direction of the specimen is lower than that within the A2, A3, and A4 ranges, indicating that the damage at the middle of the rock sample is considerably greater than at the upper and lower ends after the peak strength. The reason for this phenomenon is related to the end of the numerical model as the loading end. Along the radial direction of the rock sample, the number of failed contact force chains shows a nonlinear increasing trend from the inside out, but the number of failed contact force chains in the R4 range is larger than that in the R5 range. This is because under confining pressure, some particles within the R5 range are squeezed into the R4 range.

Furthermore, after the peak strength of the rock sample, the number of failed contact force chains near the unloading surface of the rock sample increases with increasing confining pressure. This microscopic response suggests that higher confining pressures can enhance lateral constraints and vertical axial compression resistance of the rock samples, i.e., under higher lateral constraints and axial pressure, it is more conducive to stress adjustment inside the rock sample, resulting in an increase in the number of failed contact force chains. Consequently, higher confining pressures result in more extensive damage and fractures in the rock samples during the unloading process.

3.3. Particle Displacement Response Characteristics

The displacement changes in particles within different regions during the loading and unloading process of rock samples are indicative of their macroscopic deformation at a microscopic level, with the magnitude of these changes directly reflecting the extent of damage and fracture in the loaded rock samples. Utilizing the data from Section 3.1, the average displacement components of particles in various axial and radial regions of the rock sample were calculated, revealing the change curves of these components throughout the loading and unloading process under different confining pressures, as illustrated in Figure 9. Positive axial displacement indicates an upward movement of particles along the model's axis, whereas negative values represent a downward movement. Similarly, positive radial displacement signifies the outward movement of particles along the radial direction of the model.

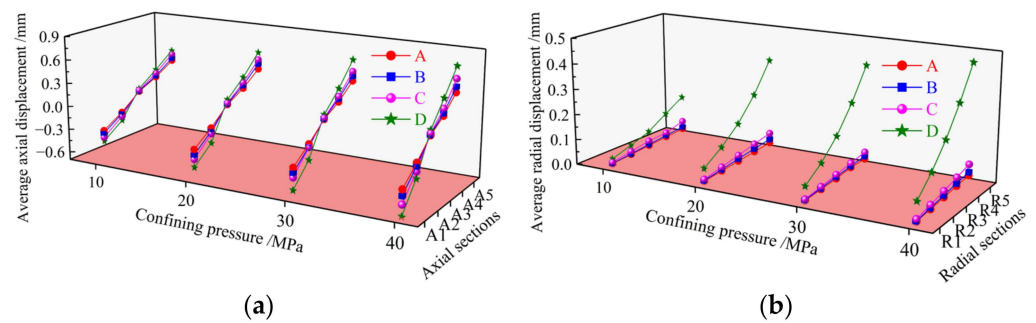


Figure 9. Trends in average particle displacement components across different regions under various confining pressures. (a) Average axial displacement components of particles in different regions. (b) Average radial displacement components of particles in different regions.

During the loading and unloading process, the average axial displacement components of particles in the rock sample's axial regions exhibit larger displacements at the upper and lower ends and smaller displacements at the middle (Figure 9). The average radial displacement components of particles across different radial regions demonstrate a nonlinear increasing trend, becoming more pronounced with higher confining pressures, particularly beyond the loading and unloading peak strength. This trend is associated with the loading end conditions of the rock sample and suggests that higher confining pressures exert stronger lateral constraints on the rock sample compared to lower pressures. With equivalent rates of unloading confining pressure, the duration of unloading is longer under higher pressures, facilitating more comprehensive stress adjustment among particles and resulting in greater axial and radial deformation of the rock sample. This indicates that higher confining pressures lead to more ductile macroscopic deformation of the rock samples from a microscopic perspective.

Additionally, Figure 9 demonstrates that under varying confining pressures, the average maximum axial and radial displacement components of particles at point C (peak strength) are ~2.61 and 1.66 times greater, respectively, than those at the initial point A of unloading; at point D, these components are ~2.81 and 14.86 times greater, respectively, compared to point A. This highlights that, from a microscopic viewpoint, the rock sample predominantly undergoes axial compression deformation before peak strength and primarily undergoes radial expansion deformation after reaching peak strength.

3.4. Particle Velocity Response Characteristics

In the PFC, the presence of frictional forces between particles in the numerical model results in minor changes in particle velocity during the application of external loads. Despite the typically low values of particle velocity, it is influenced by the external loading environment, meaning that for different confining pressures, the velocity response of particles within the rock sample will vary under identical loading conditions.

Utilizing the numerical test data from Section 3.1, the average velocity components of particles in various axial and radial regions of the rock sample were calculated. These calculations facilitated the derivation of change curves for the average velocity components of particles in different regions throughout the loading and unloading process under varying confining pressures, as illustrated in Figure 10. In the figure, positive axial velocity values indicate an upward movement of particles along the model axis, whereas negative values denote a downward movement. Similarly, positive radial velocity values represent the outward movement of particles along the model's radial direction.

As depicted in Figure 10, when compared to a confining pressure of 10 MPa, the maximum mean velocity components of particles at point C under a confining pressure of 40 MPa are ~0.91 times (axial) and 0.87 times (radial) those in the corresponding region at the lower pressure. At point D, the maximum mean velocity components under a confining pressure of 40 MPa are ~0.51 (axial) and 0.61 (radial) times those at the lower pressure.

This pattern indicates that during the loading and unloading process, particle velocity in different regions decreases with an increase in confining pressure, particularly after the peak strength. This decrease is attributed to the fact that under low confining pressure, the lateral constraint on the rock samples is relatively minimal, allowing for more active particle movement compared to conditions of high confining pressure. However, this increased particle activity does not necessarily lead to effective stress adjustment between particles, resulting in less expansion deformation than under higher confining pressures.

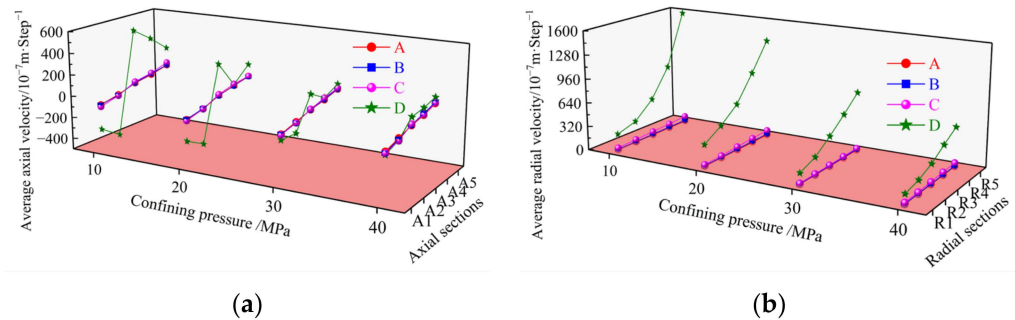


Figure 10. Trends in average particle velocity components across different regions under various confining pressures. (a) Average axial velocity components of particles in different regions. (b) Average radial velocity components of particles in different regions.

Additionally, particle velocity near the unloading surface exhibits notable variation with different confining pressures, with lower pressures resulting in higher velocities. This behavior suggests that the lower the confining pressure, the more unfavorable it is for stress adjustment between internal particles in the rock sample.

3.5. Evolution Characteristics of Cracks

The numerical model in PFC, comprising particles and bonding materials between them, allows for the simulation of the fracture evolution process in rock samples by representing the damage to bonds between particles as microcracks. Figure 11 displays the evolution curves of microcracks during the loading and unloading process of diorite rock samples under various confining pressures.

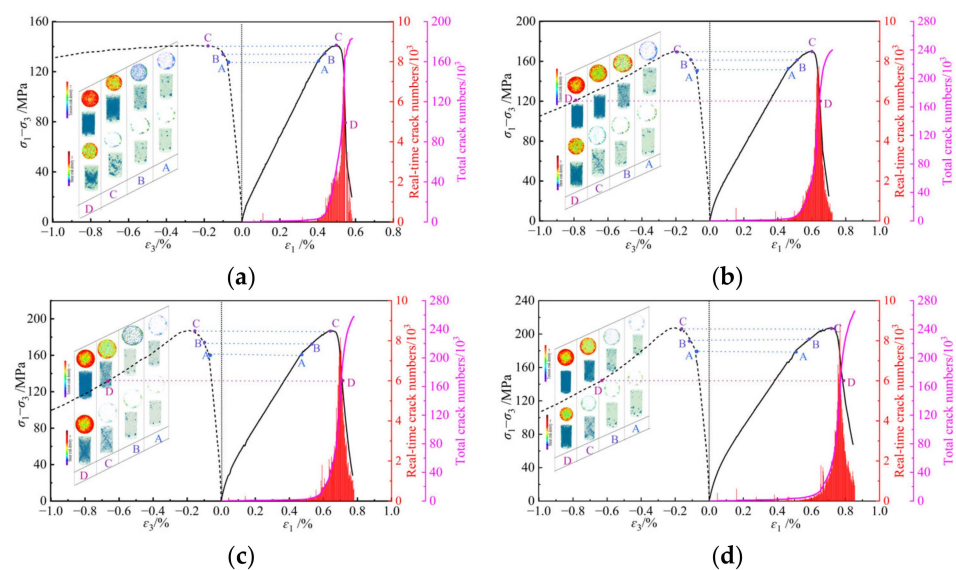


Figure 11. Evolution of microcracks during the loading and unloading process in the rock samples under different confining pressures: (a) 10 MPa; (b) 10 MPa; (c) 30 MPa; (d) 40 MPa.

Analysis of Figure 11 reveals that prior to unloading confining pressure (before point A) and during the A-to-B stage of unloading, the total number of microcracks in the rock samples remains relatively low, with a random spatial distribution. In the B-to-C stage of unloading, the total number of microcracks begins to increase rapidly, with internal microcracks developing and expanding predominantly near the unloading surface. Tensile cracks are distributed evenly along the axial direction of the rock sample, and shear cracks concentrate at the sample's shear zones. Following the peak strength of loading and unloading (after point C), the rock samples' load-bearing capacity declines sharply, and the number of real-time microcracks peaks before rapidly decreasing. As the process approaches point D, internal microcracks continue to expand and penetrate, leading to a further increase in the total number of cracks, which then gradually stabilizes beyond point D.

Furthermore, Figure 11 shows that under confining pressures of 10, 20, 30, and 40 MPa, the numbers of microcracks within the rock sample are 1.83×10^5 , 2.39×10^5 , 2.54×10^5 , and 2.65×10^5 , respectively, indicating a trend of gradual increase. Hence, as confining pressure increases, the number of microcracks increases, exacerbating the damage and fracture severity of the rock sample under loading and unloading conditions. During unloading, microcracks predominantly concentrate near the unloading surface, with shear cracks accumulating near the macroscopic failure shear surface and tensile cracks considerably outnumbering shear cracks. This suggests that under different confining pressure conditions, the fracture evolution of rock samples during loading and unloading is primarily characterized by a tensile shear failure mode.

4. Conclusions

Herein, numerical tests were performed to examine the microscopic response characteristics of diorite rock samples against the macroscopic deformation of diorite rock samples under four different confining pressures, yielding the following conclusions:

- With a constant unloading rate, higher initial confining pressures enhance the rock samples' load-bearing capacity. The confining pressure strength curve displays instantaneous fluctuations during unloading, becoming more pronounced with increased initial confining pressures. This suggests that the internal damage of the unloaded rock samples progresses through sudden expansions.
- A decrease in initial confining pressure leads to higher particle velocities near the unloading surface but results in reduced particle displacement components, contact force chain failures, and total internal microcracks. Microscopically, this indicates that the internal damage and fracture of the rock sample are relatively weak under low confining pressure conditions.
- Throughout the unloading process, the number of tensile cracks in the rock samples surpasses that of shear cracks, with tensile cracks primarily located near the unloading surface. This indicates that the fracture evolution of rock samples under varying confining pressures is predominantly characterized by tensile shear failure, highlighting the critical role of tensile mechanisms in the loading and unloading fracture process.

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Conflicts of Interest: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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