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Preliminary communication

Investigating the effect of layering and schistosity on the mechanical behavior of rocks using the discrete element method

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Abstract

Anisotropy and deformation in rock material is mainly caused by the non-uniformity and irregular geometry of fracture systems. This factor is among the important problems in designing and evaluating the stability of engineering structures. In this research, the mechanical behavior of layered and schistose rocks is investigated by conducting compressive uniaxial and triaxial strength laboratory tests on rock samples from different directions and angles varying with respect to the loading axis. The tests were carried out on intact blocks of quartz schist rock with 0° layering and invisible schistosity. Next, numerical modelling was performed using the discrete element method (DEM) and calibrating numerical models by laboratory tests. In this process, three types of connections between the minerals (i.e. mica-mica, mica-quartz, and quartz-quartz), the growth of cracks, and the fracture mechanism of layered rocks with different layering angles were investigated. The results showed that unlike the arrangement of the rock particles, the layering angle of quartz schist has an important effect on the mechanical properties of the rock in such a way that uniaxial compressive strength, Young's modulus, cohesion, and internal friction angle respectively have the greatest effect due to the change of the layering angle, while the tensile strength has the least effect.

Keywords:

Quartz schist; calibration; schistosity surfaces; discrete element method; mechanical properties of rock

1. Introduction

The effect of rock layering on the deformation and fracture resistance is controlled by the rock type, anisotropy nature, and the parallelism degree of the planes of weakness. Most rocks have anisotropic properties due to the presence of layering and other weak parts. Over millions of years, due to mechanical, chemical, or thermal phenomena, these rocks may become heterogeneous and behave inhomogenously. Information about anisotropic rocks can have wide geological applications. In general, anisotropy can be found in different scales in a rock environment, from intact samples to the entire rock mass (**Chen et al., 1998; Dehghan et al., 2015a**). Based on the process involved in the formation of weak surfaces, anisotropy is divided into two groups: inherent and induced. In the inherent heterogeneities, the emergence of weak levels is related to the stages of rock formation structure, such as the layering surface and schistosity that are formed during the steps after the sedimentation of the rock. While induced inhomogeneities are formed due to the application of subsequent stresses in the region examples of induced inhomogeneities include joints, faults, and fractures in the ground (**Guo, P., 2006; Dehghan et al., 2015b; Dehghan et al., 2017a; Farsimadan et al., 2020**). The effect of anisotropy is shown in the degree of permeability, cohesion, tensile strength, and friction coefficient of rock samples. Studies conducted around rocks show that parameters that quantify pore irregularities have similar distributions, and their values indicate the high complexity of the pore geometry, which can significantly impact permeability (**Pavičić et al., 2021**). In general, metamorphic rocks have the highest degree of anisotropy due to the formation of layers with different mineralogical compositions. In these rocks, the thermal gradients and pressures caused by tectonic activities have created schistosity surfaces in these rocks, leading to their anisotropic behavior (**Liao and Amadei, 1991; Chen et al., 1998**). When a rock is subjected to tension, it may fail along weak anisotropic planes such as bedding, seams, faults, and schistosity. Therefore, due to the high importance of anisotropy in all stages of designing engineering structures, extensive

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studies have been conducted to better understand this behavior and investigate its role in crack propagation. The research conducted by Donat et al. (1964) on slate rocks is one example of the studies conducted around the discussion of anisotropy; Also, Gray (**1967**), Otto Sanford (**1974**), studied the anisotropy of phyllite and schist rocks. Studies conducted by Briševac et al. (**2021**) showed that Regression tree models, while using parameters of uniaxial compressive strength and point load index, make it easy to estimate the modulus of elasticity (**Homand et al., 1993; Kwaśniewski, 2006; Akram and Sharrock, 2010; Bidgoli and Jing, 2014; Fuenkajorn and Klanphumeesri, 2010; Dehghan et al., 2016a; Dehghan et al., 2016b; Dehghan and Khodaei, 2017b; Aladejare and Wang, 2019; Dehghan, 2020, Briševac et al., 2021**).

One method to investigate the effect of layering in rock samples is to perform laboratory tests (triaxial compressive strength, uniaxial and Brazilian tensile test) which are performed on the rocks in different directions. Also, one of the tools for analyzing anisotropy and investigating its effect on the mechanical properties of rock is the use of numerical methods. Numerical methods are powerful tools for studying the rock fracture mechanism by calibrating their outputs with laboratory test results (**Bahaaddini et al., 2019; Lee et al., 2001**). Thus, in this research, laboratory samples were numerically simulated in PFC2D software to investigate the rock fracture process and mechanism. As one of the most widely used DEM-based computer programs, PFC2D has been successfully used in a wide range of engineering applications, such as the simulation of intact rocks, rock fractures, and underground rock retainers (**Huang, 1999; Kaitkay, 2002; Lei and Kaitkay, 2002; Tannant and Wang, 2002; Potyondy and Cundall, 2004; Akram and Sharrock, 2010; Deisman et al., 2010; Mas Ivars et al., 2010; Asadi et al., 2012; Bahaaddini et al., 2013; Bahaaddini et al., 2014; Bahaaddini et al., 2016; Bahaaddini et al., 2017; Jiang et al., 2018; Cui et al., 2019; Khodaei et al., 2021a; Khodaei et al., 2021b; Khodaei et al., 2021c**). In this software, intact rock is simulated as a set of particles (round in PFC2D and spherical in PFC3D) that are connected to each other at contact points. A major characteristic of the software is the ability to simulate, create, expand, and merge cracks explicitly. These features make this software a powerful tool for understanding the process of rock fracture mechanism under different loading regimes (**Huang, 1999; Ismael et al., 2014; Wang et al., 2018**).

To our knowledge, the flat joint method has been studied less and researched for rock mechanic problems than other existing methods. Hence, in this research, schistose rocks are modelled numerically using this method. The flat joint model simulates the macroscopic behavior of a linear, banded, and frictionally connected joint that can be partially damaged.

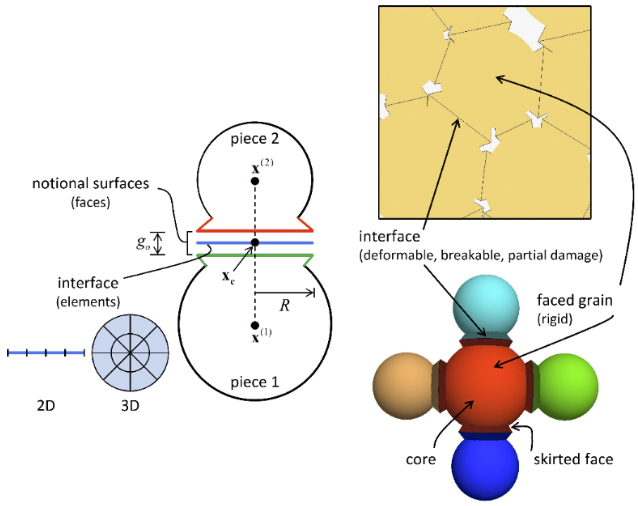

Figure 1: Schematic view of the flat joint model (Huang, 1999)

The behavior of a joint elastic element is linear. When the applied force exceeds the strength of the bond, the bond breaks, and the behavior of the elastic element is linear after failure. In this method, each element can withstand the applied force and moment (**Bahaaddini et al., 2019**). In this model shown in **Figure 1**, two hypothetical surfaces are placed at the point of contact of the balls with each other, thereby giving a skirt-like shape to the end of the particles. The contact point is a flat line in two-dimensional mode and a flat surface in three-dimensional mode, which can be divided into a few radial and peripheral elements. These bonded or non-bonded elements can be frictional.

The present study aims to study the mechanical behavior of layered rocks and consider the importance of this issue which follows the ISRM recommendations. To this end, the behavior of quartz-schist layered rocks with different layers has been investigated and simulated using the DEM numerical simulation. In this research, the behavior of layered rock is investigated through numerical modelling and calibrating it with laboratory results in 0° layering for three types of connections between the minerals constituting this rock and layering varying from 0 to 90°.

2. Material and methods

In this study, the effect of layering angle on the mechanical behavior of rocks was investigated on an intact sample of quartz schist from the Kouh Nimeh copper mine. Next, the fracture mechanism and mechanical behavior of quartz schist are investigated by conducting laboratory tests of uniaxial and triaxial compressive strength on the rock sample with 0° layering. In other words, the model used is calibrated with a zero-degree layered rock sample, and then the mechanical properties of the rock in other layers are predicted by PFC software, and there is no need to prepare samples and laboratory studies at all angles. Finally, it is calibrated with numerical models to examine the mechanical behavior of quartz schist.

2.1. Preparation of samples

The analyses and investigations related to layered rocks were performed on the quartz schist rock of the Kouh Nimeh copper mine (Ariana Mineral Industrial Company, Mountain Mine) located in the Delfard region, south of the Kerman Province in Iran. Quartz schist rock is mainly composed of mica and quartz, with the latter being more highly resistant than mica (**Kargl, 2011**). According to **Figure 2**, in order to create a laboratory sample, after performing the fire process in this mine, the rock is converted into smaller blocks and in the laboratory, in order to conduct studies from the rock blocks, coring has been done. In the sample preparation stage, the goal was to prepare cores with a diameter of 54 mm and a height of 115 mm from quartz schist rock with zero-degree layering for laboratory studies. **Figure 3** shows the method of coring from the quartz schist rock mass. Due to the limitations of costs and the number of samples, laboratory studies were conducted at a zero-degree angle and after confirming the studies, more modelling was conducted at different angles. The results of the numerical and laboratory studies on the zero-degree layered rock sample confirm each other and after verification, the rest of the models were made at different angles.

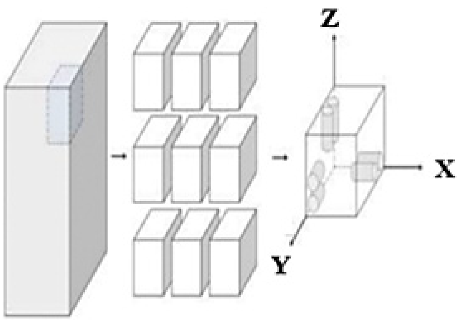

Figure 2: Coring method (Jafari Mohammadabadi, 2021).

2.2. Laboratory studies

After sampling and creating cores from intact blocks of quartz schist with 0° layering with respect to the horizon, a set of laboratory tests were carried out as uniaxial compressive strength (UCS), triaxial compressive strength (with lateral pressures of 2, 4, and 6 MPa), and the Brazilian tensile strength test which follow the ISRM recommendations. As can be seen in **Figure 4**, in the triaxial compressive strength test, the quartz schist sample is broken diagonally to the upper base and has a brittle behavior and according to the way of breaking, most cracks were shear cracks. In addition, the results of laboratory studies are shown in **Tables** 1 and **2**.

2.3. Numerical study

In numerical modelling, the aim is to investigate the initiation and growth of cracks that break in an oval or cylindrical shape, so the elastoplastic modulus is considered. Before modelling in PFC2D software, it is necessary to determine the properties of microparameters. However, since the properties of particles and the bond between them differ from the large-scale behavior of rocks, determining microparameters is among the major challenges. Generally, these parameters are obtained through the calibration process. In this method, the microparameters are selected to reach the laboratory-measured mechanical properties. The first stage of the calibration is to obtain the modulus of elasticity (E), and the second stage is to obtain the Poisson's ratio (ν) of the

Figure 3: Sample preparation; a) quartz schist mass; b) coring; c) prepared core.

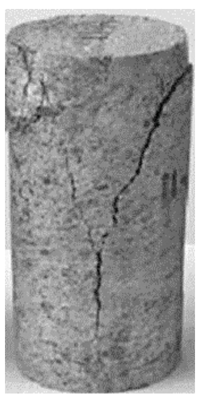

Figure 4: The failure mode of the quartz schist rock sample with 0° layering

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Table 1: The results of laboratory studies on quartz schist layered rock with a layering angle of 0°

Test	Lateral pressure (MPa)	Length (mm)	Surface area (mm)	Force (kN)	Stress (MPa)
Uniaxial compressive strength (UCS)	0	108	2289.06	137	59.84
Triaxial compressive strength	2	108	2289.06	218	95.23
Triaxial compressive strength	4	108	2289.06	235	102.66
Triaxial compressive strength	6	108	2289.06	269	117.51

Table 2: Properties of quartz schist layered rock with 0-degree layering angle

Property	Value
Young's modulus (GPa)	33
Brazilian tensile strength (MPa)	6.65
Cohesion (MPa)	11.11
Internal friction angle (°)	53.17

Table 3: Calibration values of microparameters of rock particles

Mineral name	Tensile strength (MPa)	Cohesion (MPa)	Friction ratio	Internal friction angle (°)	Young's modulus (GPa)	K_n/K_s	Number of surfaces elements	Bonded fraction ratio	Minimum radius (mm)	Maximum radius (mm)	Density of particles (kg/m³)
Mica	13	85	0.08	10	7.3	3	4	0.86	0.4	0.6	2900
Quartz	10	75	0.08	8	2.4	2	4	0.86	0.4	0.6	2900
Contact	7	30	0.02	5	0.7	2	4	0.86	0.4	0.6	-

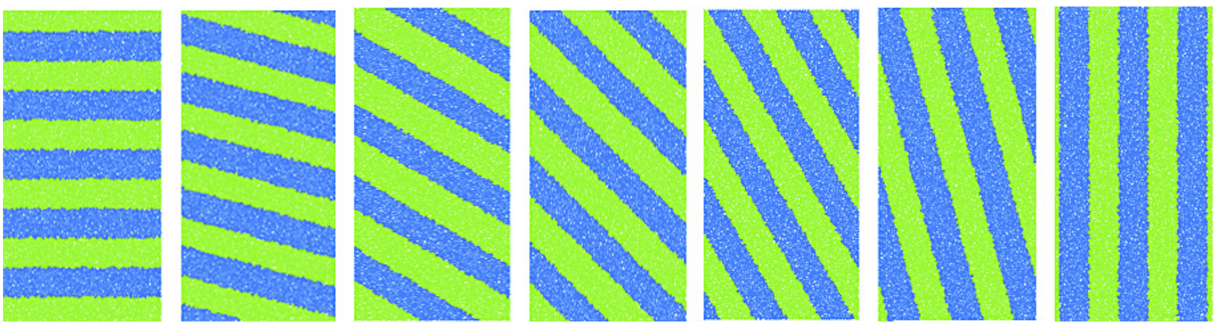

Figure 5: Numerical models made of quartz schist in PFC software with the following layering: a) 0°; b) 15°; c) 30°; d) 45°; e) 60°; f) 75°; and g) 90°.

material. Since both parameters show the material deformation, the first and second steps are performed recurrently, and the strength parameters of the material are calibrated with UCS values (**Kargl, 2011**). The calibrated values of the microparameters for the quartz schist rock sample are presented in **Table 3**, and the built models are shown in **Figure 5**.

3. Results

After conducting laboratory and numerical studies on the sample of layered quartz schist rock with 0° layering with respect to the horizon, numerical and laboratory results were compared to validate the numerical method (see **Table 4**). The output indicates that the numerical models were calibrated by the laboratory test. Therefore, the mechanical behavior of the quartz schist rock with different layers can be examined using the constructed models.

After confirming the laboratory studies by numerical modelling in 0° layering, the results of UCS, triaxial compressive strength, and Brazilian tensile tests were compared in PFC2D software. According to **Figure 6**, more modellings were performed in 0, 30, 15, 45, 60, 75, and 90° layering to investigate the behavior of layered rock to investigate the failure mode of this rock sample. The different arrangements of particles in this software affect the permeability and porosity of the built models and increase the accuracy of numerical studies. For this reason, in order to investigate the effect of particle displacement on the strength and deformation of the samples and increase the accuracy and check the accuracy of numerical studies, three types of particle arrangement have been considered and averaged.

As can be seen in **Figure** 6, changes in the layering angle affect the way the rock breaks in such a way that at an angle of 0 degrees, the rock is in the most resistant state and at an angle of 90 degrees, due to the alignment

Table 4: Comparison of the results of numerical and laboratory tests for layered schist quartz rock with 0° layering

Test type	Tensile strength (MPa)	Internal friction angle (φ; °)	Cohesion (c; MPa)	Young's modulus (v; GPa)	Uniaxial compressive strength (MPa)
Laboratory tests	6.65	53.17	11.11	33	59.84
Numerical studies	6.77	53.8	10.54	32.3	57.5

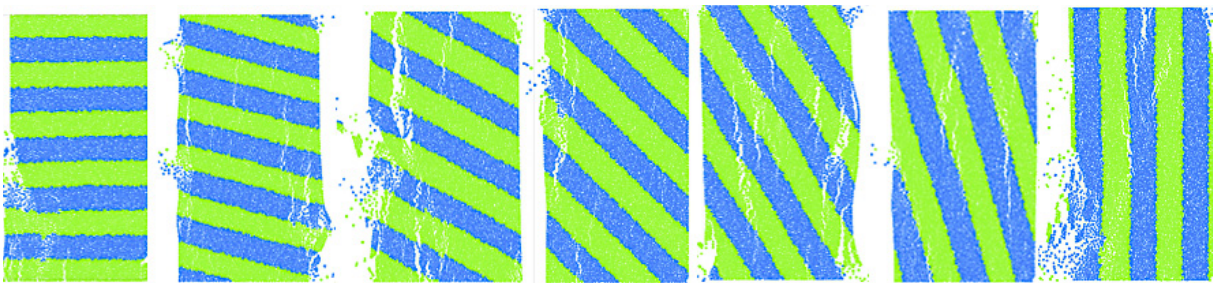

Figure 6: Failure mode of layered schist quartz rock with different layering angles: a) 0°; b) 15°; c) 30°; d) 45°; e) 60°; f) 75°; and g) 90°.

of the weak layering link with the load axis, the resistance of the sample is reduced, and it breaks easily. In other words, the elastic and dynamic properties of rocks change with changes in the layering angle.

4. Discussion

In this research, with the aim of investigating the effect of layering and schistosity on the mechanical behavior of rocks, a set of laboratory tests including uniaxial compressive strength test, triaxial compressive strength test and Brazilian tensile test were performed on quartz schist layered rock samples with a layering angle of 0 degrees with respect to the horizon. In order to increase the accuracy of the laboratory studies, each of the mentioned tests has been performed 4 times, and finally 12 laboratory tests have been performed on the sample of zero grade quartz schist layered rock. After conducting

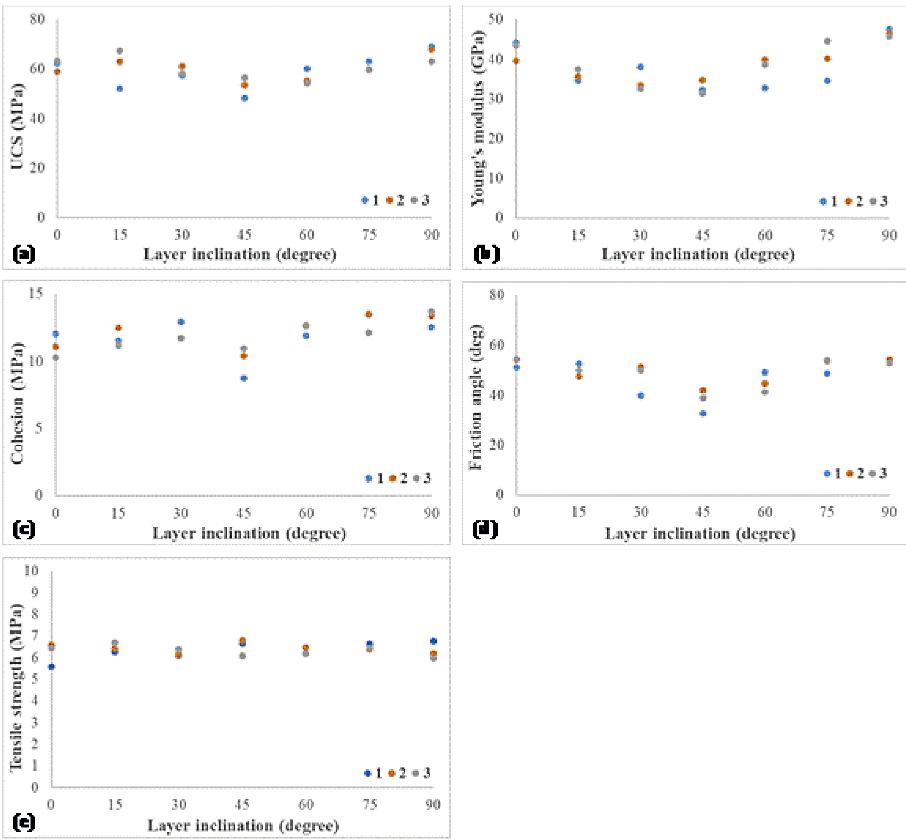

Figure 7: Sensitivity analysis for the properties of the layered quartz schist rock with respect to layering angle: a) Uniaxial compressive strength (UCS), b) Young's modulus, c) Cohesion, d) Friction angle, and e) Tensile strength.

numerical studies and simulations with the PFC software, it was found that the results of the numerical studies and the laboratory studies on zero-degree stratification of quartz shale are similar and confirm each other. Therefore, to predict the rock behavior, sensitivity analysis was done based on the verified model. According to **Figure 7**, the curves of each of the parameters of uniaxial compressive strength (UCS), cohesion, Young's modulus, friction angle and tensile strength are drawn according to the change in the slope of the layers, and the behavior of the rocks is investigated. The effect of three different types of particle arrangement to increase the accuracy of numerical studies is shown in the graphs of **Figure 7**. According to this figure, the different arrangement of particles in numerical modelling does not have a significant effect on the results of studies and can be ignored. Also, in this figure, the influence of layering angle on the mechanical properties of quartzite rock has been investigated. According to **Figure 7a** the effect of layering with different angles on uniaxial compressive strength has been investigated. As it is clear in the relevant diagram, the resistance of the rock sample is at its lowest at the layering angle of 45 degrees, and if the layering angle of the rock is 90 degrees, this parameter is at its maximum value. Also, in the diagram of **Figure 7b** the effect of rock layering angle on Young's modulus has been investigated. According to this figure, as the layering angle increases from 0 to 45 degrees, the value of this parameter decreases, and from 45 to 90 degrees, the Young's modulus of quartz schist increases again. Also, the estimation of the modulus of elasticity. The results of their studies showed that petrographic characteristics are very important and directly affect the physical and mechanical properties and the modulus of elasticity (**Briševac et al., 2021**).

The changes in cohesion according to the rock layering angle are shown in **Figure 7c**. According to this figure, while the layering angle changes, at the angle of 45 degrees, the value of the cohesion parameter is the lowest and at the angle of 90 degrees, this parameter is at its maximum value. **Figure 7d** shows the changes in the friction angle according to the rock layering angle and with the increase of the rock layering angle from 0 to 45 degrees, the value of the friction angle decreases and from 45 to 90 degrees, the value of this parameter will increase. The lowest effect of changes in the rock layering angle can be seen in **Figure 7e** on the tensile strength parameter. With changes in the layering angle, this parameter shows less fluctuations than other parameters, i.e. changes in the layering angle have very little effect on the tensile strength of the rock sample.

4. Conclusions

The mechanical properties of layered rocks are a function of their layering angle. In this respect, previous studies used one type of connection between particles in studying these properties. However, the present study preliminarily investigated the mechanical behavior of layered quartz schist rock while examining three types of connection between the layered rocks. In this research, the mechanical behavior of layered rock with layering angles of 15, 30, 45, 60, 75, and 90° was investigated by conducting laboratory studies on intact rock samples with 0° layering angle and numerical model calibration. In general, the main results of this study can be outlined as follows:

- Layering is a weak structure in the quartz schist rock, and changes in the layering angle affect the rock's mechanical properties. It has been established that it had the greatest effect on Young's modulus and the least effect on tensile strength.
- At an angle of 45° degrees, the mechanical properties of quartz schist, including young's modulus, uniaxial compressive strength, cohesion, friction angle, and tensile strength, are lower than other angles. Also, these properties are at their highest value at the 90° angle compared to other angles.
- The strength and deformation anisotropy of fractured rock environments is an important issue for designing and evaluating the stability of engineering structures. Based on preliminary investigations into the mechanical behavior of layered quartz shale rock from Iran, it was tentatively established that the anisotropy is mainly due to the non-uniformity and irregular geometry of the fracture systems.
- The samples of quartz schist rocks were considered anisotropic due to the existence of fracture systems with different angles; Therefore, the behavior of the rock is variable in different loading directions.
- For now, it has been established that the arrangement of particles does not have a significant effect in conducting numerical studies and is ignorable.
- The discrete element method (DEM) is a suitable tool for simulation of the mechanical behavior of intact layered rocks. However, simulations can generally and in no case replace the performance of tests and the estimation of the physical and mechanical properties of the rock material.

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SAŽETAK

Istraživanje utjecaja slojevitosti i škriljavosti na mehaničko ponašanje stijena metodom diskretnih elemenata

Anizotropija i deformacije u stijenskome materijalu uglavnom su uzrokovane neujednačenošću i nepravilnom geometrijom loma. Ti čimbenci čine jedan od važnih problema u projektiranju i procjeni stabilnosti inženjerskih konstrukcija. U ovoj studiji istražuje se mehaničko ponašanje uslojenih i škriljastih stijena provođenjem laboratorijskih ispitivanja jednoosne tlačne ćvrstoće i čvrstoće u trosnome stanju na uzorcima stijena iz različitih smjerova i kutova koji se razlikuju u odnosu na os opterećenja. Ispitivanja su provedena na intaktnim uzorcima kvarcne stijene sa slojevitošću od 0° i manje uočljivom škriljavosti. Zatim je provedeno numeričko modeliranje metodom diskretnih elemenata (DEM) uz kalibraciju numeričkih modela na osnovi laboratorijskih ispitivanja. U tom procesu istražene su tri vrste veza između minerala (tj. tinjac – tinjac, tinjac – kvarc i kvarc – kvarc), progresija pukotina i mehanizam loma slojevitih stijena s različitim kutovima slojevitosti. Rezultati su pokazali da kut slojevitosti kvarcnoga škriljevca ima važan učinak na mehanička svojstva stijene za razliku od rasporeda čestica stijena. Tako da jednoosna tlačna čvrstoća, Youngov modul, kohezija i unutarnji kut trenja imaju najveći učinak zbog promjene kuta slojevitosti, a vlačna čvrstoća ima najmanji učinak.

Ključne riječi:
kvarcni škriljac, kalibracija, škriljavost površine, metoda diskretnih elemenata, mehanička svojstva stijene

Author's contribution

Mahdi Aftabi (1) (PhD candidate) carried out the laboratory experiments, numerical simulation and provided analyses, writing, presentation and interpretation of the results. **Kaveh Ahangari (2)** (Full Professor at the Faculty of Engineering) proposed the key ideas and contributed to the methodology, interpretation, and analyses of the results. **Ali Naghi Dehghan (3)** (Assistant Professor at the Faculty of Engineering) managed the whole process and supervised it from the beginning to the end.