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Numerical Simulation of Mineral Composition Effect on Thermal Cracking of Rock

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ABSTRACT

Many geo-engineering applications, such as geothermal energy extraction and underground nuclear waste storage, lead to significant temperature variations. When rock is undergone through temperature increase, many cracks would be generated due to the thermal cracking process as shown in literature and laboratory experiments. These microcracks can have beneficial or detrimental impacts depending on specific application. Different thermal expansion coefficients of various mineral particles are considered as the key factor affecting the thermal cracking of rocks. In order to understand the thermal cracking process and evaluate and select the potential site for different applications, numerical simulations on thermal cracking of rocks were conducted with discrete element method. The variations of elastic modulus, tensile strength and thermal expansion coefficient with temperature were considered in the simulation. Based on the mineral analysis of granite sample from a hot dry rock well in Lijin of China, three main mineral particles, namely quartz, K-feldspar and plagioclase feldspar, were included in the numerical simulation. The simulation shows that the ratio of mineral composition plays an important role in thermal cracking besides the thermal expansion coefficient difference. When the proportion of quartz, K-feldspar and plagioclase feldspar changes from 1:1:8 to 4:4:2, the statistical cracks increase approximate ten-fold. The more one of mineral compositions is, the less the thermally produced microcracks are. The more the two minerals with the largest difference of thermal expansion coefficients are, the more the thermally produced microcracks are. It means that the rock with more complex mineral compositions has a high probability of thermal cracking.

1. INTRODUCTION

Rock is a heterogeneous material composed of different minerals with different geometry and dimension of pores and microcracks. When rock undergoes thermal load, the phenomenon of thermal cracking or thermal fracturing will occur due to the thermal stress (Liu et al., 2018). Under such conditions, some new cracks will be created along mineral grain boundaries and/or through mineral grain, and/or pre-existing microcracks will be activated to re-open and propagate (Géraud, 1994). Many experimental and theoretical works have been done to try to understand thermal cracking. A widely accepted mechanism for thermal cracking is that minerals in continuously heated rocks have different thermal expansion (or contraction) coefficients, which expand at different rates and induce strain at the grain boundaries and then inter-granular cracking (Cooper and Simmons, 1977; Davidge, 1981; Fredrich and Wong, 1986; Homand-Etienne and R., 1989; Lin, 2002; Liu et al., 2001; Mene´ndez et al., 1999). Thermal load will cause dramatic temperature changes in the rock and result in variation of rock stress and rock properties due to volumetric contraction or expansion.

Bauer and Handin (Bauer and Handin, 1983; Bauer and Johnson, 1979) had measured the thermal expansion of various water-saturated heated rocks under different effective confining pressures. Microcrack developments have been observed from 25 oC to 800 oC, which are associated with thermal expansions of minerals. Mineralogy is well-known to play a key role in rock thermal damage or thermal cracking. With the increasing of temperature, the crystal particles of rock generate new microcracks between mineral grains because of differential thermal expansion among different grains which have different thermal properties, such as thermo-elastic moduli and thermal conductivities (Dmitriyev et al., 1972; Heard and Page, 1982; Kranz, 1983). Differences of thermal expansion between different minerals cause crack nucleation and increase the crack density in rock. David et al.(David et al., 2012) showed that the crack density of La Peyratte granite increased from 0.16 at room temperature to 0.86 at 600 oC temperature. There is a dramatic increase of crack density of La Peyratte granite between 500 °C and 600 °C because of α–β transition of quartz occurring at 576 °C.

The experiments and observations mentioned have distinctly showed that mineralogy has an important effect on thermal cracking. Although the thermal cracking process under different thermal loading conditions can be captured in laboratory using Acoustic Emission or Scanning Electron Microscope, numerical modeling is an alternative and useful way to understand the influence of mineral content on thermal cracking as it cannot be observed with laboratory experiment. This paper proposes a numerical model for studying the effects of minerology on rock thermal cracking process based on elastic damage mechanics, thermal-elastic theory and the discrete element method. The changes of rock's thermal properties with temperatures are also considered in the simulation. A physical model is built based on the main mineral components analyzed from a Lijin granite sample with by X-ray. The proposed model is then implemented with bonded-particle approach. Finally, the effects of mineral composition ratio on crack number, crack propagation and pore evolution in rock are discussed.

2. THERMAL-MECHANICS MODEL FOR THERMAL CRACKING

The rock interior re-structuring caused by thermal load is a thermal-mechanical coupling process. This process can be modelled and simulated with Particle Flow Code (Li and Soliman, 2014; Wanne and Young, 2008). The fundamental idea is to introduce a

thermal strain by changing the size of particles, and then introducing thermal stress into the mechanical contact model, to model the numerical simulation of the thermal cracking (Itasca, 2008).

The heat conductivity through the contact surface of two particles is given by:

$$Q_c = H_c(T_i - T_j) \tag{1}$$

$$H_c = h_c A = 2 r_c \gamma_p \tag{2}$$

Where, T_i and T_j are temperatures of the adjacent two particles, °C; H_c is the heat transfer coefficient on particle contact surface under unit time and temperature difference, J/K; A is the contact area between two particles, m^2; r_c is the contact radius of particles, m; λ_p is the thermal conductivity coefficient of particles, W/(m·K).

In the particle flow simulation, thermal interactions are usually treated as a network of heat reservoirs (associated with particles) and thermal pipes (associated with contact surfaces) (Fig. 1). Heat flow between two heat reservoirs (particles) occurs through the thermal pipes (contact surfaces) by heat conduction. By modifying the particle radius and the force of the parallel bond, the thermal strain is generated to simulate the thermal load process.

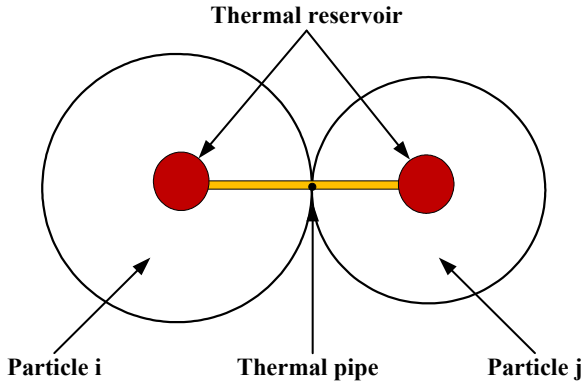


Figure 1 Thermal contact model

Assuming that the strain change no effect on the temperature, the thermal energy balance of a 1D continuum can be derived and expressed by:

$$-\frac{\partial q_i}{\partial x_i} + q_v = \rho C_p \frac{\partial T}{\partial t} \tag{3}$$

where, q_i is the heat flux vector, w/m^2; q_v is the volumetric heat source intensity or power density, w/m^3; ρ is the mass density, kg/m^3; C_p is the specific isobaric heat capacity, J/(kg·K); T is the temperature, °C; t is the heating time, s; x_i is the displacement of i^{th} particle, m.

The relationship between heat flux and temperature gradient can be defined by continuous Fourier heat conduction law and given as:

$$q_i = -k_{ij} \frac{\partial T}{\partial x_j} \tag{4}$$

where, k_{ij} is the thermal conductivity tensor, w/(m·K); x_j is the displacement of j^{th} particle, m.

When particle is subjected to thermal load, its volume will change with temperature variation. The thermal strain can be modeled as follows:

$$\Delta R = \alpha R \Delta T \tag{5}$$

where, ΔR is change in particle radius caused by thermal load, m; α is the linear thermal expansion coefficient of particle, $1/K$; R is the particle radius, m; ΔT is temperature difference between two adjacent particles, K.

Considering that a bonded linear parallel bond is present at the mechanical contact associated with a thermal contact, the expansion of the bond material can be calculated by assuming that only the normal component of the force vector carried by the bond will be affected by the temperature change. The isotropic expansion of the bond material can be modeled by changing the normal component of the bond force vector as:

$$\Delta \overline{F}^n = -\overline{k}^n A(\overline{\alpha} \overline{L} \Delta T) \tag{6}$$

where, $\Delta\overline{F}^n$ is the normal component of the bonding force vector, N; $\overline{k}^n$ is the bond normal stiffness, N/m^3; A is the area of the bond cross-section, m^2; $\overline{\alpha}$ is the linear thermal expansion coefficient of bonding material, 1/K; $\overline{L}$ is the bond length between the centroids of two adjacent particles, m.

3. PARAMETERS FOR NUMERICAL SIMULATION

3.1 Mineral Components and Numerical Specimen Model

A granite sample was taken from a well drilled in a hot dry rock reservoir located in Lijin County, China. X-ray diffraction analysis method was used to analyze mineral components. The rock sample consists of about 28% quartz, 17% K-feldspar, 48% plagioclase feldspar, 2% calcite, 2% ferrodolomite and 3% clay and other tracing minerals. Given that the interior structure and morphology of a rock are determined by the main components of minerals in thermal cracking process, which results in different thermal cracking threshold for different rocks (Fredrich and Wong, 1986; Homand-Etienne and R., 1989; Zhang et al., 2007; Zhang and Zhao, 2009). Therefore, quartz, K-feldspar and plagioclase feldspar are considered in the study. Figure 2 depicts the segmented image revealing the morphology of the three minerals in granite. The numerical specimen is 55 mm in length and 25 mm in width. The grain diameter ranges between 0.6 mm and 0.8 mm. Total 3517 grains are included in the numerical specimen. The linear thermal expansion coefficients of quartz, plagioclase feldspar and K-feldspar are taken as 15×10^{-6} K^{-1}, 13×10^{-6} K^{-1} and 11×10^{-6} K^{-1}, respectively (Fei, 1995).

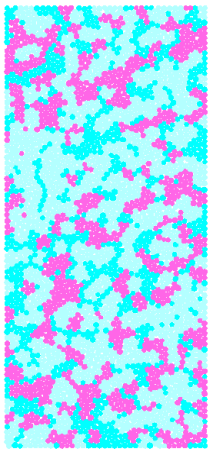


Figure 2: Distribution of minerals in numerical specimen of granite generated by PFC^{2D} with cluster model. The quartz, K-feldspar and plagioclase feldspar minerals are shown as magenta, cyan and light-cyan color, respectively.

3.2 Thermal Properties of Granite and Numerical Model Parameters

A lot of studies showed that the rock thermal properties would change with temperature (Sang et al., 2001; Somerton and Selim, 1961; Xu et al., 2013). With the increasing of temperature, the elastic modulus and strength of granite decrease, and the linear thermal expansion coefficient increases. Such changes in macro scale affects the thermal cracking process. Therefore, it is necessary to consider the changes of these thermal properties in numerical simulation. Xu et al. (Xu et al., 2013) conducted experiments on granite under uniaxial compression at temperatures varying from 25 to 850 °C to study the effect of temperature on rock strength and deformation. Curve fitting on these experiments yielded the following correlations as shown in Eq. (7) – Eq. (9).

$$\alpha(T) = 7.715 \times 10^{-7} \times e^{T/209.70} + 6.41 \times 10^{-6} \quad (7)$$

$$\sigma_c(T) = 115.439 + 151.668 \times e^{-T/51.236} - 14.717 \times e^{T/631.292} \quad (8)$$

$$E(T) = 1.289 + 207.229 \times e^{-T/11.911} + 12.019 \times e^{-T/871.270} \quad (9)$$

where, α is the linear thermal expansion coefficient of granite, °C^{-1}; σ_c is the compressive strength of granite, MPa; E is the elastic modulus, GPa; T is the heating temperature, °C.

Other parameters used in the PCF^{2D} model for granite specimens in this work are listed in Table 1.

3.3 Heating Process

The different coefficient of linear thermal expansion is assigned to different minerals before heating. The temperature changes by 5 °C every step to minimize the effect of thermal shocks (Richter and Simmons, 1974). Considering the effect of α-β phase transition in quartz particle, the radius expansion with 1.0046 is applied when temperature increased to 573 °C, and the radius contraction with 0.9954 is adopted when temperature decreases to 573 °C (Carpenter et al., 1998). The whole numerical specimen is heated to simulate the rock heating process in a high temperature muffle furnace. The temperature changed from 25 °C to 800°C at a step of 100 °C. At each temperature, the numerical specimen was maintained at the temperature for two hours.

3.4 Simulation Scenarios

The heterogeneity of rocks indicates the uniformity of mineral distribution. The smaller the heterogeneity is, the larger the proportion of certain minerals in the rocks is, and the more uniform the physical properties of rocks tend to be. According to the mineral analysis results of granite sample, 12 scenarios of different mineral proportions among three mineral components of quartz, K-feldspar and plagioclase feldspar were designed to characterize the heterogeneity of rocks, as shown in Table 2. According to the

changes of main mineral component, they are divided into 3 groups. In group A, the quartz content gradually increases. In group B and group C, the contents of plagioclase feldspar and K-feldspar gradually play a key role. The mineral distributions for each scenario are shown in Fig. 3.

Table 1 Microscopic parameters of granite used in cluster model

parameter	unit	value
Density	kg/m^3	3000
Coefficient of thermal conductivity	W/(m·K)	2.5
Porosity	%	0.5
Heat capacity	J/(kg·K)	1015
Contact stiffness ratio	/	2.0
Damping coefficient	/	0.7
Friction coefficient	/	0.5
Contact normal strength	MPa	60
Contact normal strength deviation	MPa	10
Contact tangential strength	MPa	60
Tangential contact strength deviation	MPa	10

Table 2 Scenarios of different mineral proportions

Mineral percentage/ %	A				B				C			
	A1	A2	A3	A4	B1	B2	B3	B4	C1	C2	C3	C4
Quartz	20	40	60	80	40	30	20	10	40	30	20	10
K- feldspar	40	30	20	10	40	30	20	10	20	40	60	80
Plagioclase feldspar	40	30	20	10	20	40	60	80	40	30	20	10

4. SIMULATION RESULTS AND DISCUSSIONS

4.1 Quartz Domination

Fig. 4 shows the distributions of microcracks in numerical specimen for each scenario of A group after 600 °C heating. Fig. 4 shows microcracks mainly occur at the contact point of quartz and K-feldspar. The microcrack type includes intergranular crack and intragranular crack. Because the linear thermal expansion coefficient of quartz is larger than that of K-feldspar, the transgranular crack mainly appears in the interior of K-feldspar. With the increasing of temperature, the amount of microcracks increases due to inducing of larger thermal stresses. Higher temperature promotes the propagation and connection of small cracks, which in turn form larger and longer cracks. With the increasing of quartz proportion in rock, microcracks induced by thermal stress firstly increase and then decrease. When the quartz proportion in rock is up to 80%, few microcracks are generated. These are related with the mineral content in rock. The larger the mineral proportion is, the more the homogeneity of rock will be and the smaller the total thermal stress induced by different minerals is. Therefore, when one mineral becomes the overwhelming majority of rock, the thermal cracking will be weakened. The statistical results of microcracks under different heating temperature are presented in Fig. 5. It can be seen that the threshold temperatures for four scenarios are all around 400 °C. Therefore, it can be inferred that the mineral with largest linear thermal expansion coefficient dominates the thermal cracking process when such mineral is the majority in rock.

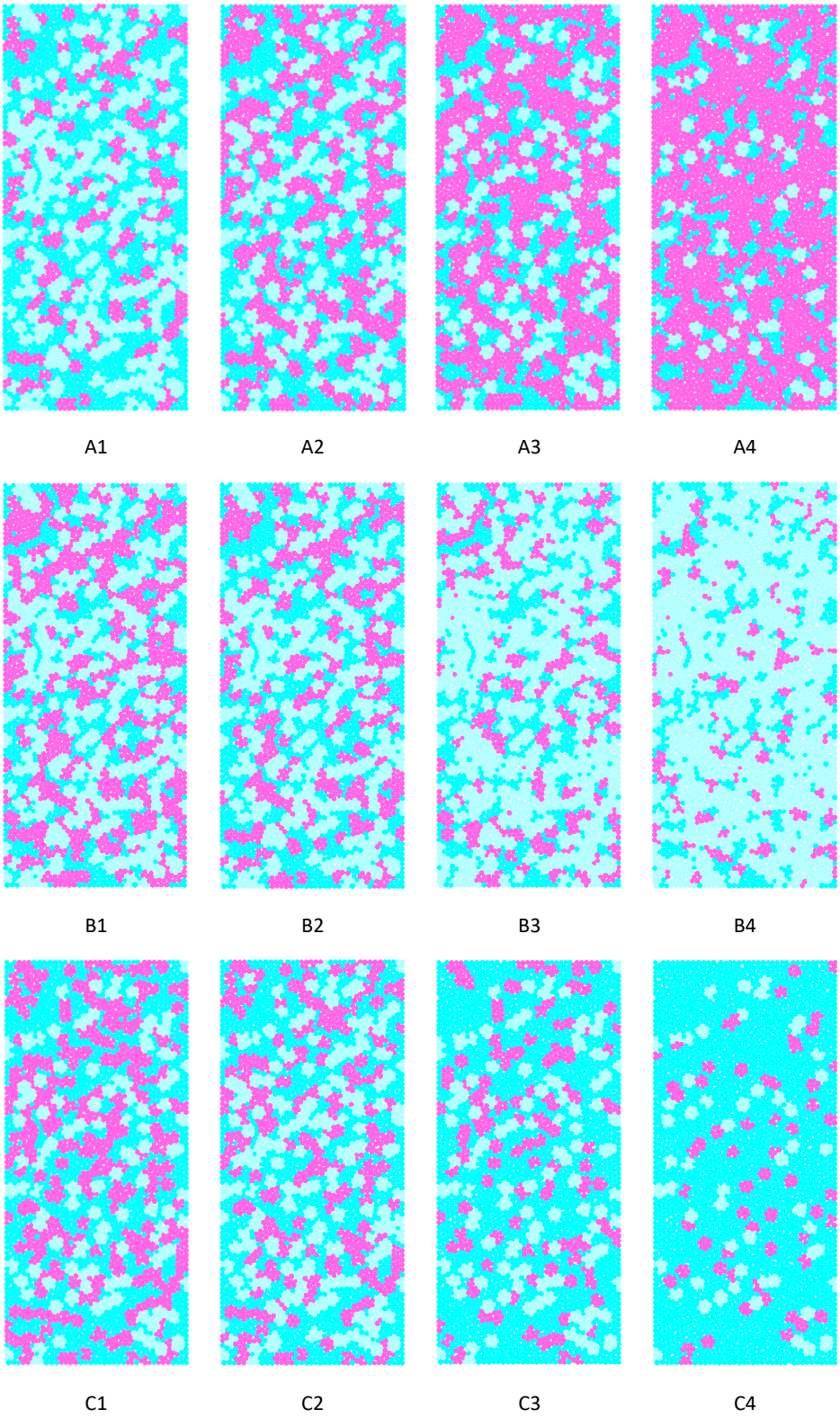


Figure 3: Mineral distributions for each scenario

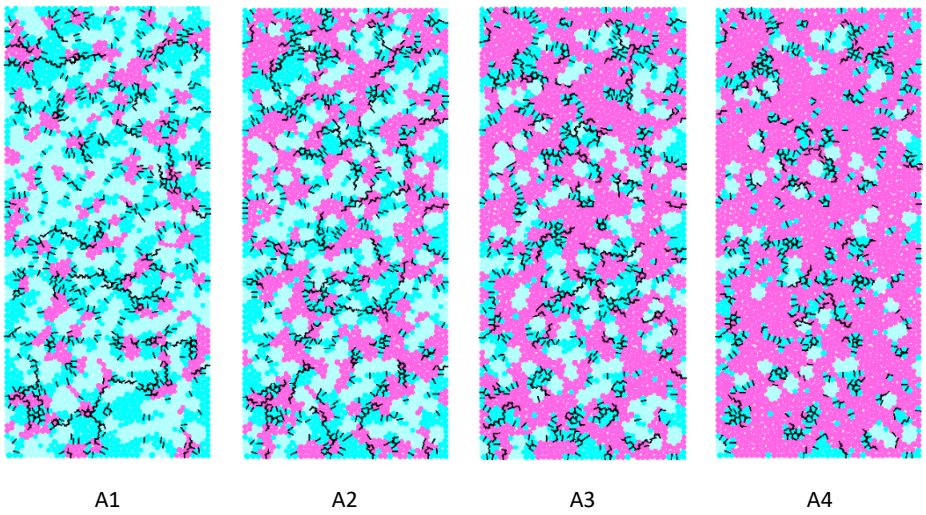


Figure 4: Crack distributions for A group scenarios after heated at 600 ºC

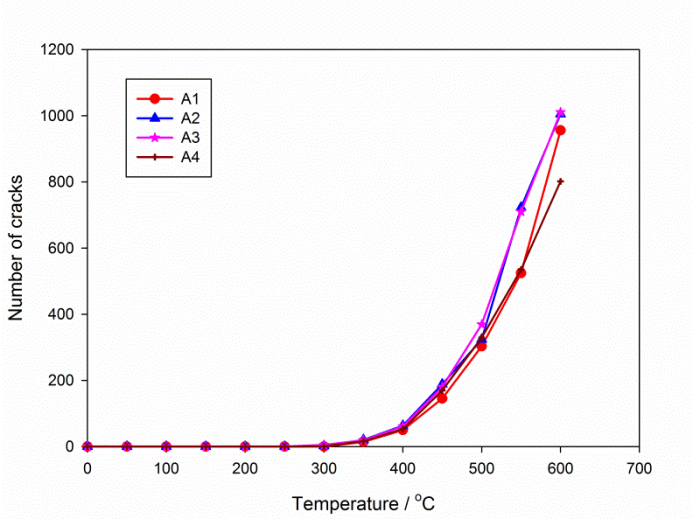


Figure 5: Number of cracks for A group scenarios after heated at 600 ºC

4.2 Plagioclase Feldspar Domination

Fig. 6 shows the distributions of microcracks in numerical specimen for each scenario of B group after 600 ºC heating. It can be seen that the most microcracks were created when the proportion of quartz, K-feldspar and plagioclase feldspar is 20:40:40 (B1 scenario). The microcrack development with mineral contents is same as quartz domination scenarios (A group). With the increasing of the plagioclase feldspar proportion, the microcracks and linear fractures decrease sharply. When the plagioclase feldspar proportion is up to 80% (B4 scenario), there are a few scattered cracks in the specimen. Fig. 7 shows the crack number changing with heating temperature for different mineral proportions. With the increasing of plagioclase feldspar, the thermal threshold temperature decreases gradually. When the proportion among quartz, K-feldspar and plagioclase feldspar is 20:40:40, the thermal threshold temperature is about 350 ºC. However, this value becomes around 500 ºC when the proportion of quartz, K-feldspar and plagioclase feldspar is up to 10:10:80. With the increasing of plagioclase feldspar, the proportion of the two minerals (quartz and K-feldspar) with the largest difference in linear thermal expansion coefficient decreases, the total number of thermally induced microcracks also gradually decreases. It indicates that the mineral content play a key role in thermal cracking process. When the total proportion of the two minerals with largest difference in linear thermal expansion coefficient becomes smaller and smaller, the thermal threshold temperature gradually increase with the increasing of other minerals with medium thermal expansion coefficient. Additionally, when the total proportion of the two minerals with largest difference in linear thermal expansion coefficient becomes larger and each proportion is nearly equal, thermal cracking will be more prominent, and the new-created cracks and fractures will increase remarkably as shown in B1 scenario. When the proportion of quartz, K-feldspar and plagioclase feldspar changes from 1:1:8 to 4:4:2, the statistical cracks increase approximate ten-fold.

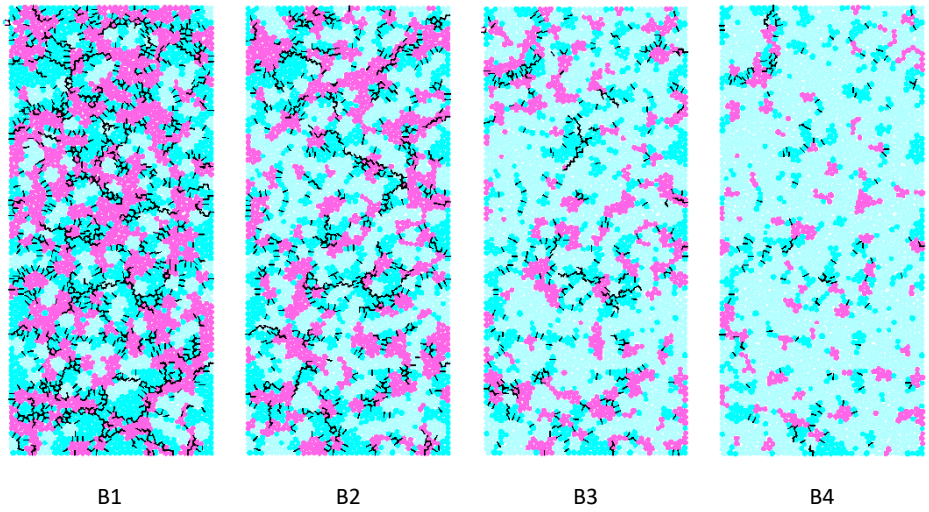


Figure 6: Crack distributions for B group scenarios after heated at 600 ºC

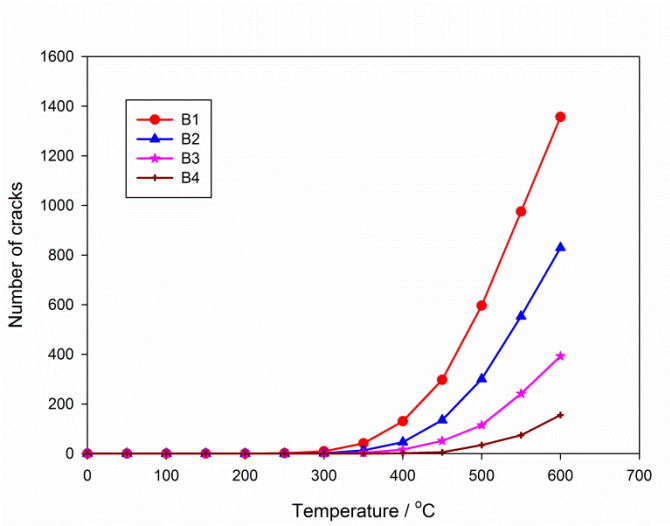


Figure 7: Number of cracks for B group scenarios after heated at 600 ºC

4.3 K-Feldspar Domination

Fig. 8 shows the distributions of microcracks in numerical specimen for each scenario of C group after 600 ºC heating. The microcracks are mainly generated in the interior of K-feldspar and the contact position between K-feldspar and quartz. With the increasing of K-feldspar proportion, the number of large linear fractures increases and more transgranular fracture are produced as shown in C3 and C4 scenarios. When the proportion of quartz, K-feldspar and plagioclase feldspar is 10:80:10 (C4 scenario), there has more linear fractures than other scenarios due to the interaction and penetration of microcracks around the quartz clusters. When the proportion of quartz, K-feldspar and plagioclase feldspar is 40:20:40 (C1 scenario), the thermal cracking are mainly happened in the interior of K-feldspar and the microcrack number is relatively smaller. The inferred thermal threshold temperatures for four scenarios are around 400 ºC as shown in Fig. 9. Again, when the total proportion of the two minerals with largest difference in linear thermal expansion coefficient occupies a dominant level and each proportion is closer, more microcracks will be induced as shown in C2 and C3 scenarios.

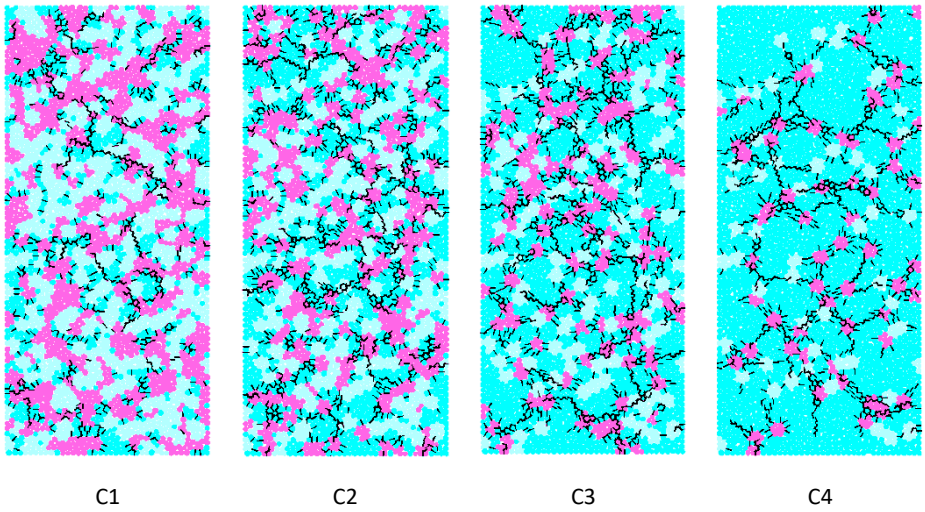


Figure 8: Crack distributions for C group scenarios after heated at 600 ℃

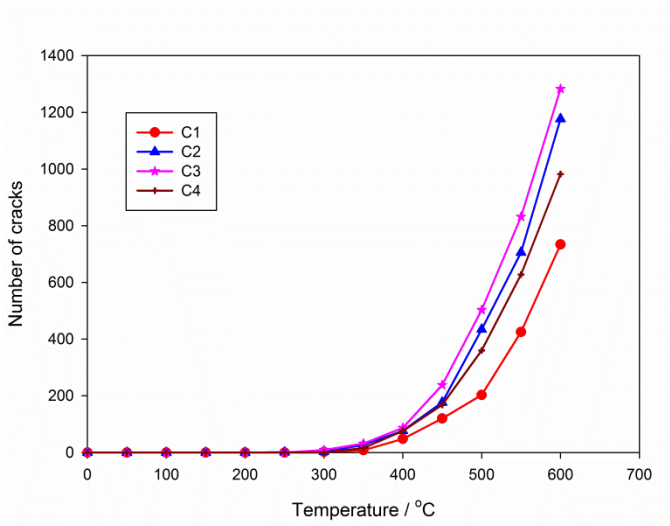


Figure 9: Number of cracks for C group scenarios after heated at 600 ºC

5. CONCLUSIONS

In this paper, the thermal cracking of rock with different minerals is numerically simulated by the discrete element method. The variations of elastic modulus, tensile strength and thermal expansion coefficient with temperature are considered in simulations. The influence of mineral composition on thermal cracking of rock at high temperature was studied. The numerical simulations show that the difference of linear thermal expansion coefficient and the mineral proportion play a dominant role thermal cracking. When a mineral occupies the majority of the rock, the rock thermal cracking happens less. Meanwhile, thermal cracking is also closely related to the proportion of minerals. When the proportion of quartz, K-feldspar and plagioclase feldspar changes from 1:1:8 to 4:4:2, the statistical cracks increase approximate ten-fold. The more one of mineral compositions is, the less the thermally produced microcracks are. The more the two minerals with the largest difference of thermal expansion coefficients are and the closer each mineral content is, the more the thermally produced microcracks are. It means that the rock with more complex mineral compositions has a high probability of thermal cracking. Therefore, the reservoirs with large difference of linear thermal expansion coefficient among minerals will be the best candidate for implementing thermal stimulation.

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