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Three-dimensional DEM investigation of the fracture behaviour of thermally degraded rocks with consideration of material anisotropy

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Abstract

A complete understanding of the fracture behaviour of anisotropic rocks under elevated temperatures is fundamentally important for rock and reservoir engineering applications. This paper shows a three-dimensional numerical investigation of the fracture behaviour of anisotropic sandstone, with consideration of the effects of temperature and material anisotropy. In the study, a 3D semi-circular bend (SCB) model was established by using the Discrete Element Method (DEM). The thermal responses of different minerals and the strength anisotropy of incipient bedding planes were considered in the model. The DEM model was calibrated against a series of laboratory experiments on Midgley Grit sandstone (MGS) that exhibits intrinsic anisotropy. The pure mode I, mode II, and mixed-mode (I+II) fracture characteristics of the MGS were investigated under elevated temperatures (up to 600 °C) using the established DEM model. The thermal degradation (i.e., fracturing) of the rock, the fracture load, the evolution of micro-cracks, and the stress-strain relationship around notch tips were analysed, with emphasis on enlightening the micro-mechanisms underlying the fracture behaviour. The results of the study were discussed and then compared with experimental observations and theoretical predictions.

Keywords

Anisotropic rock; Temperature; Fracture behaviour; Discrete Element Method; Rock discontinuity

Nomenclature

A_b	the cross-sectional area of parallel bond
a	notch length
B1-B5	five bedding planes with different strengths
C_v	specific heat
CMTSS	conventional maximum tangential stress criterion
d, d_1, d_2, d_3, d_4	different bed spacings
DEM	Discrete Element Method
EGS	enhanced geothermal system
GASED	generalized average strain energy density
GMTSN	generalized maximum tangential strain criterion
GMTSS	generalized maximum tangential stress criterion
ISRM	International Society for Rock Mechanics and Rock Engineering
K_{Ic}, K_{IIc}, K_{Eff}	mode I, mode II and mixed-mode fracture toughness
k_n	parallel bond normal stiffness
L	bond length
LR	loading rate
MGS	Midgley Grit sandstone
P_f	fracture load
PFC	Particle Flow Code
R	radius of SCB specimen
r	particle radius
s	half of the support spacing in three-point bending tests
SCB	semi-circular bend
T	temperature
T^-	T^- stress in SCB specimens
t	thickness of SCB specimens
TPB	three-point bending
Y_I , Y_{II}, T^*	dimensionless geometry factors
α	linear thermal expansion coefficient

α_b	the linear expansion coefficient of bond material
α_p	the coefficient of linear thermal expansion
β	inclination of pre-existing notch
γ	thermal resistance
∇F	thermal force acting on parallel bond
∇r	change of particle radius
∇T	temperature increment

1. Introduction

A better understanding of the fracture characteristics of anisotropic rocks in high temperature environment is fundamentally important for many rock and reservoir engineering applications such as disposal of high-level radioactive waste [1-3], and design of hydraulic fractures for EGS [4]. The fracture of a rock material takes place when the stress intensity factor at the crack tip reaches a critical value, which is termed as fracture toughness. Fracture toughness is a crucial parameter of a rock material that describes its fracture behaviour and ability to resist fracturing [5]. This parameter is often used in fracture prediction [6] and reservoir stimulation control [7-8].

Previous investigations on fracture behaviour of rocks showed that fracture toughness can vary with factors like temperature, pressure [9-11], material anisotropy [12-13], geometrical properties of tested samples [14-15], experimental setup and the loading conditions [16]. Therefore, the rock fracture behaviour is complex and often difficult to be fully understood. However, there is a consensus that rock fracture toughness can increase under elevated temperatures until it reaches an elasto-plastic transition phase [17], after which a decrease can be expected [12,18-20]. The transition phase is rock type-dependent, and depends on mineralogy. De Castro lima and Paraguassu [21] pointed out that the increase in thermal expansion coefficient can be up to 20% when the quartz content for granitic rock is increased.

The process of fracture initiation and propagation is markedly affected by rock material anisotropy, which mainly arises from: (1) complex geological formation (due to the existence of irregular pores, flaws, unequally-cemented layers, and unevenly-distributed micro-cracks, etc.), and (2) thermally- or mechanically-induced cracks that increase the degree of heterogeneity. For anisotropic rocks with pre-existing cracks, fractures may not propagate smoothly as expected for the case of isotropic rocks but instead arrest due to the pre-existing cracks [22] and sometimes divert into anisotropic planes [13, 23]. Na et al. [24] presented a numerical investigation on the fracture initiation and propagation of layered shale under Brazilian tests, and revealed that fractures can initiate, propagate and coalesce in many ways due to the presence of anisotropic layers. Lee et al. [25] experimentally demonstrated how the mechanically-induced fracture interacted with pre-existing discontinuities (mineral veins) in notched SCB shale samples. Three typical fracture patterns were observed in their study: (1) crossing the veins with a slight deflection from planar path, (2) diversion along veins, and (3) fracture initiation at the side of the notch (rather than the notch tip), jogging, and propagation along the veins.

Geological bedding planes may have different strengths due to various diagenetic (various deposition and sedimentation rates) and environmental (weathering, unloading) conditions. However, the fracture complexity of anisotropic rocks stemming from the bedding strength anisotropy is not well understood, and associated studies are rare in literature. This is mainly due to the fact that the incipiency of a discontinuity is extremely difficult to be fully reflected in the current experimentations, and the sampling of natural rocks and sample preparation are always uncontrollable (the incipiency of a discontinuity refers to the relative tensile strength of that of parent rock [26, 27]). It is extremely difficult to obtain a group of natural rock samples containing discontinuities with controllable incipiency [28]. The role of discontinuity incipiency has only been associated with how it affects fracture behaviour in only one previous study [29]. However, only limited surrogate discontinuities were prepared and tested in that study. This limitation can be overcome by numerical techniques.

The main objective of this study was to investigate the effects of temperature and material anisotropy on the fracture behaviour of anisotropic sandstone through the Discrete Element Method (DEM). The semi-circular bend (SCB) setup suggested by ISRM [30] was used for that purpose. The micro-mechanisms underlying the fracture behaviour of the anisotropic rock under temperature and loading were explored. The effects of bed spacing and relative bed position on the fracture load and effective fracture toughness were discussed. A review of available studies of the temperature effect on fracture toughness was then reported, followed by discussion, and comparison of the results of the present numerical study with theoretical predictions**.**

2. Thermo-mechanical scheme and SCB sample genesis

2.1 Thermo-mechanical scheme used in the study

In this study, the Particle Flow Code (PFC 3D) was used to mimic the thermo-mechanical behaviour of rocks. This section briefly describes of the thermo-mechanical scheme implemented in the PFC 3D. A detailed description of the code is given in [31].

The thermal algorithm available in the PFC 3D allows the consideration of the thermal expansion of both the bonded particles and the parallel bonds by assigning different timescales to the mechanical and thermal processes [31]. Note that in the current PFC 3D algorithm, only the parallel bond model can consider thermal expansion, not the bonds defined with the smooth joint contact model. The thermal force (∇F) acting on the parallel bonds under high temperatures was only accounted for at the normal contact direction, without considering the bond lateral expansions, such as [31]:

$$\nabla F = -k_n A_b \alpha_b L \nabla T \tag{1}$$

where k_n is the parallel bond normal stiffness, A_b is the cross-sectional area of the parallel bond, α_b is the linear expansion coefficient of the bond material which is the average value of the expansion coefficients of the particles connected by the bond, L is the bond length, and ∇T is the temperature increment.

In the thermal process, the particles can expand under high temperatures by changing the particle radius (*r*), which is described as:

$$\nabla r = -\alpha_p r \nabla T \tag{2}$$

where α_p is the coefficient of linear thermal expansion associated with the granular particles.

2.2 Genesis of SCB sample considering material anisotropy

Fig. 1 shows the representative anisotropic SCB sample used in the study. The sample contained incipient bedding planes with different tensile strengths. The genesis of the SCB sample follows the four steps given below:

- Generation of particles ─ A group of assembly particles with a radius of 1.0-1.5 mm was generated in a semi-circular vessel with a radius (R) of 50 mm and a thickness (t) of 30 mm. The particle radius follows a uniform distribution [32]. Each particle was randomly identified as a mineral type, and four mineral groups were generated with a similar mineral composition to the MGS sandstone (i.e., 70% quartz, 10% feldspar, 15% clay and 5% biotite [27]).
- Insertion of anisotropic layers ─ Five incipient bedding planes (B1-B5) with different tensile strengths [27, 33] were inserted into the SCB sample. Note that, short transverse-oriented layers were focused in the present study, as proposed by Roy et al. [29] and Shang et al. [16].
- Supporting and loading bars ─ One loading bar (red cylinder in Fig. 1) and two supporting bars (blue cylinders, with a spacing of 55 mm) were created, following the ISRM standard (i.e., $0.5 \leq s/R \leq 0.8$ [27]). A group of particles (light green particles in Fig. 1) contacting the three bars was generated, and a zero thermal expansion coefficient was assigned to these particles to eliminate stress concentration at the bar-particle contacts during the thermal treatment.
- Generation of pre-existing notches ─ Within each SCB sample, a notch with a length (*a*) of 25 mm and an inclination (β) between 0°- 46° was generated (Fig. 1), allowing a full consideration of fracture modes for the specific combination (i.e., for the setup a/R = 0.5 and s/R = 0.55, $\beta = 0°$ represents mode I, $\beta = 46°$ mode II, and $0° < \beta < 46°$ mixed mode [16, 34]).

The generated SCB samples were first heated to the desired temperatures (up to 600 °C), before performing the three-point bending (TPB) tests by moving the loading bar at a constant loading rate (LR) of 0.001 m/s (Fig. 1).

2.3 Selection of micro-parameters and thermal parameters

The micro-parameters of the parallel bond and the smooth joint of the SCB sample have been calibrated by Shang et al. [32], by perfoming direct tensile tests on intact MGS and bedding planes (see [32] for details). Fig. 2a shows a comparison of the laboratory and DEM results; while the failure patterns of the rock samples are shown in Fig. 2b. The calibrated micro-parameters used in this study are shown in Table 1. It should be noted that tensile tests were used to calibrate the parallel bond micro-parameters, based on two reasons: (1) elimination of the intrinsic limitation of the parallel bond model that tends to overestimate the tensile strength of rock; (2) from a macroscopic point of view, the SCB samples were expected to exhibit tensile failures in the three-point-bending tests.

A set of thermal parameters including linear thermal expansion coefficient (α), thermal resistance (γ) and specific heat (C_v) were used in the study to consider thermal effects [31]. Specifically, different linear thermal expansion coefficients were assigned to the each mineral of MGS (i.e., quartz, 24.3×10^{-6} K^{-1}; feldspar, 8.7×10^{-6} K^{-1}; biotite, 1.0×10^{-6} K^{-1}; clay, 3.6×10^{-6} K^{-1} [35, 36]). The specific heat of the DEM sample and thermal resistance per unit length were 920 J/ (kg K) and 0.43 m K/W, respectively. The micro-parameters α and C_v were set equal to the macro-values of the MGS.

3. Results

3.1 Thermal degradation of rock

Fig. 3 shows the thermal response of the simulated MGS sample (β=0°) that was heated to different temperatures (20 °C ≤ T ≤ 600 °C). For clarity, the particles are not shown in the figure, only thermally induced microcracks and the five bedding planes (i.e., B1-B5) are presented. As can be seen, a few microcracks were thermally induced under relatively low temperatures ($T \leq 200$ °C). Interestingly, those microcracks clustered around the pre-existing notch. This was probably related to the creation of the pre-existing notch that has led to a mechanical degradation of adjacent rock materials. Hundreds of microcracks were induced within the rock sample when the applied temperature was increased to 350 °C, while thousands of microcracks can be seen when the temperatures were further increased to 400, 500 and 600 °C. It is noted that the failure of parallel bonds dominated under different temperatures, certainly due to the fact that only the parallel bonds can consider thermal expansion in the current PFC scheme as mentioned in section 2.1.

3.2 Thermal influence on fracture load

The temperature dependency of the fracture load in three-point-bending tests has been reported by many researchers [11, 17-20]. A consensus has been reached that the fracture load tends to increase with temperature and then decrease above a certain threshold value. As demonstrated in Fig. 4a, slight increases in the fracture loads of the isotropic MGS samples were observed for all cases (β=0° - 46°) when the temperatures were raised to ~350 °C. A further increase in temperature has led to a pronounced decrease in the fracture load. However, the decrease in the fracture load above 350 °C was not due to mineral transition as observed in the laboratory [37].

A similar relationship between the fracture load and temperature was noticed for the anisotropic MGS (Fig. 4b). It was noted that the fracture loads of the anisotropic MGS (Fig. 4b) slightly decreased compared with that of isotropic MGS (Fig. 4a). The change in fracture load between the two types of rocks was due to the presence of the five weaker bedding planes. For example, in ambient temperature, the measured mode I fracture load of the isotropic MGS was 882 kN (black dots in Fig. 4a). It increased to 1045 kN when the temperature was raised to 350 °C, and then decreased to 713 kN at a temperature of 600 °C. For the anisotropic MGS, the corresponding fracture loads were 667 (20 °C), 780 (350 °C) and 323 kN (600 °C), respectively (Fig. 4b).

3.3 Fracture complexity of anisotropic rocks having been thermally degraded

The origin of the fracture complexity of an anisotropic rock mainly arises from the interaction between the mechanically induced fractures and the pre-existing defects (i.e., pre-existing micro-cracks, anisotropic layers, and thermal cracks). A fracture deviation is often expected in anisotropic rocks. Figs. 5-7 show how the deviation occurred in the anisotropic MGS samples under different temperatures and fracture modes (i.e., mode I, mode II and mixed-mode I+II).

In these figures, the particle displacement field (in the x direction) are presented, showing positive horizontal displacements on the right side of the principal failure plane and negative displacements on the left side. For clarity, the particles are represented by the centre point; whilst the thermally induced cracks (green) and mechanically induced cracks (black) are differentiated.

As shown in Fig. 5a, a curved principal fracture plane (indicated by the yellow dashed line) was initiated from the pre-existing notch tip and diverted into the relatively weak bedding plane (i.e., B3), similarly to what was observed in a laboratory observation (Fig. 5n) [38]. The unexpected fracture plane observed in Fig. 5n implied that some factors were at play (probably the pre-existing micro-cracks that cannot be seen by the naked eye). However, the curved fracture path shown in Fig. 5a was likely due to the anisotropic layers. This hypothesis was further evidenced by the similar fracture planes shown in Figs. 5b, 5d, and 5f. Fig. 5i shows a similar fracture pattern observed in the anisotropic Mancos shale [39], where the fracture initiated from the notch tip and propagated approximately along a weaker bedding plane. A second deviation along another adjacent bedding plane was seen, leading to an “S”-shaped macroscopic failure plane.

Another interesting observation was that two curved fracture planes (all initiated from the notch tips but on the opposite side) were induced in the samples that were previously heated to 200 (Fig. 5c) and 350 °C (Fig. 5e). The generation of the twin fractures was probably related to the thermally induced micro-cracks, which were just located at the opposite side of the notch tips and promoted fracture initiation. This fracture behaviour is, however, presently difficult to be verified by experiments as it is still hard to find comparable laboratory experiments that consider both temperature and material anisotropy.

It is known that a single fracture often initiates from notch tips in TPB tests, although a secondary fracture deviation sometimes occurs (Fig. 5i). Apart from this, the specimen can also fail away from the pre-existing notch, as demonstrated in Fig. 5f. Fig. 5f shows that many micro-cracks were induced around the supporting bar. A similar rupture was observed by Wang and Yang [40] in their fracture toughness tests on a bedded coal (Fig. 5m). The mechanisms underlying the rupture are complex and there are still no consensus agreements. However, it is envisaged that the rupture can be associated with the micro-cracks or other defects (like micro-poles) present in the rock.

Fig. 6 shows the fracture characteristics of the samples under different temperatures and mixed-mode (I+II) loading (β=30°). The curved macro-fractures were initiated from the pre-existing notch tips (Figs. 6a-6e). A special feature was observed when the pre-heating temperature was increased to 400 °C, where the induced fracture diverted to the anisotropic layer B4 (Fig. 6f). This observation was similar to that found in a laboratory study performed on an artificial anisotropic sandstone (Fig. 6i, [29]). The SCB samples that were heated to a relatively high temperature (600 °C) did not show a clear macroscopic fracture plane (Fig. 6h), which was due to the widely spread thermally induced micro-cracks that markedly changed the stress condition of the rock.

Although the fracture behaviour of the samples under mode II loading (β=46° in Fig. 7) show some similarities with that of samples shown in Figs. 5 and 6, a clear difference in the fracture pattern was observed. As indicated in Figs. 7c and 7e, the mechanically induced fractures did not initiate from the notch tip, but from the intersection points of the B4 layers and the pre-existing notches. Similar experimental observations are shown in Figs. 7i and 7j [39, 41]. The main reason for this unexpected fracture pattern was due to the thermally induced cracks on the side of the pre-existing notches, which contributed to the initiation of the curved fractures.

3.4 Evolution of micro-cracks

As an example, the evolution of micro-cracks against computational step under different fracture modes (i.e., mode I, mode II, and mixed mode) is shown in Fig. 8, where the induced micro-cracks are also shown. The tensile failure of the parallel bonds dominated the three modes without exception, implying that the tested SCB samples failed in tension from the microscopic point of view (Fig. 8).

The number of micro-cracks increased gradually with computational step until reaching a critical point where a dramatic increase in the number of micro-cracks occurs.

3.5 Stress versus strain around notch tips

To understand the effect of temperature on the stress - strain relationship around notch tips, three measurement spheres (embedded in PFC 3D) with a constant radius of 7.5 mm (more than 5 times of the maximum particle radius) were used, with their centers located at the notch tips. The measured notch tip stress, strain, and displacement have three components (i.e., along the x, y and z directions), which are related to principal values. The x component of those measured values is presented considering the opening nature of the SCB samples (i.e., along the x direction).

Fig. 9 shows the calculated stress - strain curves (in the x direction) for different temperatures (*T* = 20, 300 and 600 °C). It is noted that the initial notch tip stress measured under 600 °C was not null, mainly because of the excessive expansions of the particles and bonds, which caused initial stress within the sample prior to the mechanical loading. Clear fluctuations in notch tip stress were measured until the peak values were reached. The peak notch tip stress increased slightly when the temperature was increased from 20 to 300 °C, while it decreased dramatically when the temperature was further raised to 600 °C.

4. Synthesis, comparison, and discussion

4.1 DEM model genesis

In the model genesis, we considered different strengths for the bedding planes. This feature has been largely ignored in literature and is extremely difficult to be fully reflected in the current experimentations, as mentioned in the introduction. The numerical study reported here considered the bedding plane incipiency and is expected to help us to better understand the fracture behaviour of anisotropic rocks. It can be anticipated that the displacement field (Figs. 5-7) and fracture load (Fig 4) are different, if only one bedding plane strength is considered.

In our model, each particle was randomly specified as a mineral type, and four different minerals were generated (see Section 2.1), following the main mineral composition of the targeted rock. To accurately reflect the thermal response of the rock, different thermal parameters (i.e., thermal expansion coefficient) were assigned to different minerals. This means that the particles in our model can expand differently under temperature, which can mimic to the maximum extent realistic thermal responses of real rock materials. It is expected that the results reported in the study can be affected if only one mineral type was considered.

Rock minerals have distinct structures, and the physical and mechanical properties (such as cementation or consolidation) between mineral grains can be different. For simplicity, the interparticle bond properties have not been modified to match the nature of rock minerals in this study, mainly because differentiating the bond properties between different minerals would require a tedious calibration process of the numeric model. In addition, to the best of the authors' knowledge, laboratory experiments on the quantification of the intergranular forces are rare in literature, which make the calibration even more difficult.

4.2 Bed spacing and position

Sedimentary rocks have different bed spacings due to various rates of deposition. The relative position of bedding planes can also vary due to the diagenesis (i.e., sediment transportation and deposition). For simplicity, a constant bed spacing (17.5 mm) was used in the study, which follows a general description of the tested rock [27, 32]. To understand the effects of relative bed position and spacing on fracture behaviour, five additional cases (i.e., Cases 2-6) were studied, considering different relative bed position and spacing (Table 2) following Shang et al. [32]. Fig. 10 presents the fracture load against temperature for the additional five cases. Comparing the five cases with that shown in Fig. 4, a similar evolution trend in the fracture load magnitude versus temperature was observed, irrespective of bed spacing and relative bed position. The fracture loads initially increased (slightly) until ~350 °C and then decreased dramatically. It is unsurprising that, there were clear differences in the magnitude of fracture load for different cases, and that the fracture loads in

Cases 5 and 6 (Figs. 10d and 10e) were relatively larger than those measured in Cases 2 - 4 (Figs. 10a - 10c).

4.3 Comparison of results with experimental observations

The present study also demonstrated that temperature indeed significantly affected the fracture behaviour of anisotropic Midgley Grit sandstone, in terms of fracture load (Figs. 4 and 10) and fracture complexity (Figs. 5-7). A comparison of the fracture toughness of different rocks under various temperatures is shown in Fig. 11. Note that equations (3) - (5) were used to calculate the fracture toughness for all different modes [16], as it has been verified that the influence of anisotropy has a very little influence on the stress intensity factors [42].

$$K_{i\mathrm{c}}=\frac{P_{\mathrm{f}}\sqrt{\pi a}}{2Rt}Y_i,\ \ i=\mathrm{I},\ \mathrm{II} \tag{3}$$

$$K_{\mathrm{Eff}}=\sqrt{{K_{\mathrm{Ic}}}^2+{K_{\mathrm{IIc}}}^2} \tag{4}$$

$$T^{-}=\frac{P_{\mathrm{f}}}{2Rt}T^{*} \tag{5}$$

where T^- is the T^- stress in SCB specimens, Y_{I} and Y_{II} are dimensionless geometry factors for mode I and mode II loading conditions, respectively. T^* is also a geometry factor. Values of these factors of SCB specimens depended on the notch length (a = 25 mm), span length (2s = 55 mm) as well as notch angle ($0° \leq \beta \leq 46°$), as reported by Ayatollahi and Aliha [34] and Shang et al. [16].

As illustrated in Fig. 11, the fracture toughness - temperature curves obtained from the DEM study showed a similar pattern with those derived from laboratory experiments. However, some discrepancies exists. Many rocks such as Manoharpur sandstone [17] exhibited an increase trend in fracture toughness until ~100 °C, after which their fracture toughness values decreased. This observed initial increment in fracture toughness has been attributed to thermal expansion of minerals [17], leading to the closing and compaction of pre-existing cracks and pores. The present DEM simulations performed on the clay-rich MGS showed a clear increment in mode I fracture toughness until ~350 °C (Fig. 11a), which is more close to the experimental observations made by Chandler et al. [19] on Darley Dale sandstone and by Funatsu et al. [11] on Kimachi sandstone, where continuous increments of mode I fracture toughness values were observed until 200 °C (no further data under higher temperatures). These two sandstones are also clay-rich, and the dehydration as well as dihydroxylation (which often occurs around 400 °C) of the clay minerals are expected [37], which can degrade the layer structures of clay minerals, leading to the decrease of fracture load and toughness. The compaction of the pre-existing cracks and transition of clay minerals however cannot be revealed in the current DEM model. However, a clear decrease in failure load above 350 °C was observed certainly due to the effect from the thermal cracking (see Fig. 3). A similar temperature effect (compared with laboratory observations) was observed on the fracture behaviour of clay-rich rocks.

4.4 Comparison of results with theoretical predictions

A comparison of the DEM results (in terms of $K_{\mathrm{Eff}}/K_{\mathrm{Ic}}$) of the present study with the theoretical predictions (shown in Shang et al. [16]) from four different fracture criteria is presented in Fig. 12. The derivation of the expressions ($K_{\mathrm{Eff}}/K_{\mathrm{Ic}}$) of the four criteria is available in Shang et al. [16], and will not be repeated here. As shown in Fig. 12a, the DEM results of the isotropic MGS under various temperatures matched well with the theoretical predictions. However, for the anisotropic MGS, a relatively large discrepancy was observed (Fig. 12b), especially when the notch angle was 10° (much smaller effective fracture toughness was numerically predicted). This difference can be attributed to the combined effects from temperature and anisotropy (i.e. short-transverse oriented layers). A clear discrepancy between our DEM results and theoretical predictions was noted, and this needs a reliable experimental study to testify if the classic fracture criteria can be used to assess the fracture behaviour of thermally degraded anisotropic rocks.

5. Conclusion

This paper reports a three-dimensional DEM investigation of the thermal influence on the fracture behaviour of sandstone, with consideration of material anisotropy. The thermal degradation of the rock, the fracture complexity, the evolution of micro-cracks, the fracture load, as well as the stress and strain around notch tips were considered. The results of the DEM study were compared with experimental results and with theoretical predictions.

Several conclusions can be drawn from the present study: (1) the combined effects of temperature and material anisotropy significantly affected the fracture behaviour of Midgley Grit sandstone; (2) a slight increase in fracture load was observed when the applied temperature was increased to ~350 °C, after which the number of thermal cracks increased dramatically, and the fracture load and fracture toughness reduced significantly; (3) four main fracture patterns were observed, which include single curved fracture, twin curved fractures (for mode I, T=350 °C), fracture away from the pre-existing notch tips (for mode II, T=200 °C), and rupture of rock matrix. The deviation of the fracture into anisotropic layers was often observed for the transverse oriented SCB samples, leading to fracture complexity; (4) The DEM results reported in the study agreed broadly with experimental results and theoretical predictions; (5) Laboratory fracture toughness experiments are needed to testify if the classic fracture criteria can be used to assess the fracture characteristics of thermally degraded anisotropic rocks.

Conflict of interest

We have no conflict of interests to declare

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Figure captions

Fig 1 Setup of the semi-circular bend DEM model containing bedding planes with different strengths.

Fig 2 Calibration of the DEM model [32]. (a) Comparison of the stress-strain curves obtained from laboratory experiments and the calibrated DEM model, and (b) fracture patterns of rock samples in direct tension.

Fig 3 DEM simulation of the degradation and fracture of Midgley Grit sandstone (MGS) subjected to different temperatures (particles are not shown for clarity).

Fig 4 Fracture load versus temperature in the TPB tests. (a) Isotropic MGS and (b) anisotropic MGS.

Fig 5 (a-h) Fracture characteristics of the thermally degraded SCB rocks under mode I loading (β=0°). (i-n) Experimental observations on different geo-materials (bedded coal and isotropic sandstone) under similar loading condition. Particle displacement field in the x direction is presented.

Fig 6 (a-h) Fracture characteristics of the thermally degraded SCB rocks under mixed-mode (I+II) loading (β=30°). (i-j) Experimental observations on different geo-materials (anisotropic sandstone and bedded coal) under similar loading condition.

Fig 7 (a-h) Fracture characteristics of the thermally degraded SCB rocks under mode II loading (β=46°). (i-j) Experimental observations on different rocks (Mancos shale and sandstone) under similar loading condition.

Fig 8 Evolution of micro-cracks against computational time step for the simulated rock with different modes and temperatures. (a) Mode I and T= 20 °C, (b) mixed-mode and T=100 °C, and (c) mode II and T= 200 °C.

Fig 9 (a) Notch tip stress versus strain, and (b) notch tip stress versus displacement (β=30°; T= 20, 300, and 600 °C).

Fig 10 Influence of bed spacing and relative bed position on the fracture load.

Fig 11 Fracture toughness against temperature: comparison of DEM results with experiments (from literature). (a) Mode I, (b) mode (II), and (c) mixed-mode.

Fig 12 Effective fracture toughness of Midgley Grit sandstone against notch angle: comparison of DEM results with theoretical predictions from four fracture criteria (ambient temperature). (a) isotropic rock, and (b) anisotropic rock.