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1 **Broad-spectrum fracture toughness of an anisotropic sandstone under**  
2 **mixed-mode loading**

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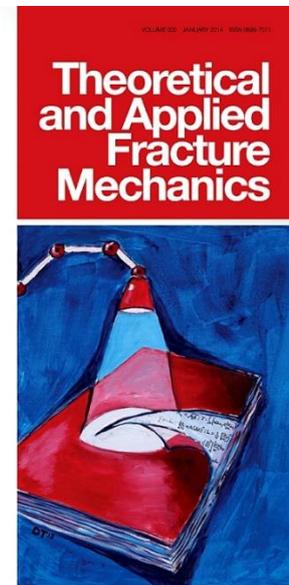
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10 Anisotropic rocks; Mixed-mode loading; Discrete  
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22 **Abstract**

23 Fracture toughness of anisotropic rocks can vary with many factors such as  
24 geological anisotropy, geometrical properties of specimens used in the  
25 laboratory (e.g., pre-existing crack properties), and loading conditions. This  
26 fact has been widely acknowledged. Yet the variation in fracture toughness  
27 remains enigmatic, as there is still lack of a comprehensive study on how  
28 those influential factors affect fracture toughness behavior of anisotropic  
29 rocks. The present paper shows a broad-spectrum mixed-mode fracture  
30 toughness of an anisotropic sandstone from a numerical scheme, which is  
31 based on the Discrete Element Method (DEM). In this study, a total of 340  
32 semi-circular bend (SCB) specimens with various geological and geometrical  
33 conditions were numerically prepared by systemically varying the orientations

34 of planar anisotropy (i.e. incipient bedding plane), as well as the magnitudes  
35 of the ISRM-suggested geometrical parameters of the SCB specimens (i.e.  
36 crack length, crack angle, and span length). The numerical model used in the  
37 study was calibrated against a series of laboratory experiments to select  
38 proper micro-parameters to reproduce the mechanical characteristics of  
39 anisotropic Midgley Grit sandstone (MGS). Additionally, four different fracture  
40 criteria, which are based on stress and strain analysis, and the analysis of  
41 energy density, were used to predict the mixed-mode fracture behaviour of  
42 MGS. Numerical findings from this study were compared with experimental  
43 observations (qualitatively) and theoretical predictions (quantitatively). A  
44 broad agreement was observed in the comparison study.

## 45 **1. Introduction**

46 Hydraulic fracturing has been widely used in the unconventional extraction of  
47 natural resources, including oil and gas and geothermal energy, for creating  
48 flow channels/fractures and enhancing permeability of tight rock formations  
49 [1]. The fracturing process will stimulate the flow of natural resources, thereby  
50 increasing the volumes that can be recovered. In the fracturing process, a  
51 controllable and predictable fracture pattern is of significant importance to the  
52 effective recovery of natural resources [2]. However, the fracture pattern can  
53 be complex and quite different for different geological settings and stress  
54 conditions, especially for fractured reservoirs with anisotropic rocks under  
55 mixed-mode loading conditions, which is therefore, difficult to be fully  
56 understood. Sustained efforts are therefore, needed for the topic.

57 Fracture toughness is an important parameter, which is used to characterize  
58 the ability of rock to resist fracturing. This parameter is often used as a  
59 criterion for predicating fracture initiation which is fundamentally important in  
60 understanding the mechanical properties of rocks. Although fracture  
61 toughness is often considered as an intrinsic property of a rock material, it still  
62 can vary with many factors including geological anisotropy [3, 4], geometrical  
63 properties of the laboratory-scale specimens [5-7], temperature [8], and  
64 loading conditions [9, 10]. As such, a comprehensive description of the  
65 possible variation of fracture toughness arising from those factors is of great

66 importance for a better understanding of the mechanical behaviour of  
67 anisotropic rocks, as well as for a proper selection of pressure and viscosity of  
68 liquid used for fracturing anisotropic rocks.

69 For transversely isotropic rocks (a typical form of anisotropy) with bedded  
70 layers (i.e., planar anisotropy), the magnitude of fracture toughness differs  
71 with respect to the relative orientation between the pre-existing cracks and the  
72 transversely isotropic bedding planes. Also, the weakness planes can divert  
73 fracture propagation, leading to a complex fracture pattern [11]. For example,  
74 Na et al. [4] numerically explored the effects of orientation and length of pre-  
75 existing cracks, as well as thickness of bedding planes on the fracture pattern  
76 of Mancos shale in Brazilian tests and concluded that geological anisotropy  
77 significantly affected fracture patterns and effective fracture toughness (EFT).  
78 It was also revealed from that study that the initiation, propagation, and  
79 coalescence of fractures within layered geo-materials depended on local  
80 heterogeneity.

81 Previous investigations on the fracture toughness of anisotropic rocks have  
82 focused on the mode I loading condition [3, 4, 12] with inadequate attention  
83 given to the mixed-mode (i.e., I+II) loading condition which is often seen in  
84 nature. Although some attempts exist [13, 14] in the study of the combined  
85 effects of geological anisotropy and mixed-mode loading on EFT, a  
86 systematic investigation is still needed since only limited scenarios were  
87 reported in previous studies. For example, Krishnan et al. [13] reported a  
88 series of fracture toughness tests on a layered sandstone under mixed-mode  
89 loading, however all tested specimens had their bedding planes perpendicular  
90 to the direction of the applied load, without considering cases with bedding  
91 planes parallel to the load direction. Roy et al. [14] reported a laboratory  
92 investigation on the mixed-mode fracture toughness of a sedimentary rock  
93 based on SCB specimens, in which the joint anisotropy (i.e., direct tensile  
94 strength) was differentiated based on the work by Shang et al. [15]. In that  
95 study, the anisotropic planes within the tested SCB specimens were oriented  
96 at a relatively small angle with respect to the loading direction, ignoring the  
97 cases with bedding planes perpendicular to the loading direction.

98 As previously mentioned, apart from geological anisotropy and loading  
99 conditions, the geometrical properties of specimens used in the laboratory  
100 also affect fracture toughness behaviour. It is known that the fracture  
101 toughness of a solid material is often measured in the laboratory and there  
102 are several suggested specimens for the fracture toughness tests, such as  
103 short rod (SR) specimen, semi-circular bend (SCB) specimen and cracked  
104 Brazilian disk (CBD) specimen [16, 17]. SCB specimens are popular among  
105 others due to the comparatively easier sample machining. A variation of  
106 fracture toughness has been observed in previous studies for SCB specimens  
107 with different crack lengths. For example, Zhao et al. [18] investigated the  
108 effect of crack length on the dynamic fracture toughness of SCB coal  
109 specimens and found that the dynamic fracture toughness of the tested coal  
110 specimens increased when the crack length was increased from 4 to 10 mm.  
111 The effect of span length on fracture toughness may also exist but research  
112 on this topic is rare.

113 The geometrical dimensions of SCB specimens have been recommended by  
114 the ISRM standard [17]. However, how the specimen dimensions within the  
115 suggested domain affect the magnitude of fracture toughness is not clear. In  
116 the laboratory measurement of fracture toughness, as a normal routine, only  
117 limited geometrical dimensions (in terms of specimen diameter, thickness,  
118 crack length and span length) of SCB specimens are used, which inevitably  
119 will lead to an incomplete description of the fracture toughness of targeted  
120 materials. Additionally, it has to be accepted that it is tedious and  
121 cumbersome for the preparation of SCB specimens in the laboratory when the  
122 influential factors described above (i.e., geological, geometrical and loading  
123 conditions) are considered simultaneously.

124 In this paper, a broad-spectrum mixed-mode fracture toughness of an  
125 anisotropic SCB sandstone was reported based on a total of 340 Discrete  
126 Element Method (DEM) simulations. The broad-spectrum fracture behaviour  
127 was achieved by systematically varying the orientation of planar anisotropy,  
128 crack length, span length, as well as crack angle in the DEM simulations. The  
129 effects of the geological and geometrical factors on fracture toughness were  
130 investigated and discussed. The effect of incipency of planar anisotropy

131 (relative tensile strength) on failure characteristic was also discussed and  
132 presented. Numerical findings in the study were compared qualitatively with  
133 previous experimental observations, and validated quantitatively against  
134 theoretical predictions.

## 135 **2. Anisotropic Midgley Grit sandstone**

136 In the study, a series of DEM simulations were performed to reproduce the  
137 mechanical characteristics of medium-grained Midgley Grit sandstone (MGS),  
138 which is produced at the Blachhill Quarry (BQ), United Kingdom (Figs. 1a and  
139 1b). The MGS is from the Carboniferous Midgley Grit Formation (Fig. 1c) and  
140 ranges from fine- to very coarse-grained sandstone [15]. The medium-grained  
141 MGS targeted in the study presents a transverse isotropy, which can be  
142 illustrated by the nicely bedded planes in a core sample (see Fig.1d). A  
143 laboratory investigation has been reported by Shang et al. [15] in the  
144 measurement of the direct tensile strength of the incipient bedding planes. It  
145 was found that the direct tensile strength of those incipient planes varied from  
146 31.3 % to 87.5 % that of intact parent rock (2.08 MPa). The MGS sample  
147 used in that study comprised 70 % quartz, 15 % clay, 10 % k-feldspar and  
148 ~5 % haematite (Fig. 1e) and the unit weight of the sample is around 22.1  
149 kN/m<sup>3</sup>. In this study, bedding planes with a direct tensile strength of 87.5 %  
150 that of parent was targeted and modelled.

## 151 **3. Numerical model setup and calibration**

### 152 **3.1 Numerical model setup**

153 Fig. 2 shows the setup of the numerical model, in which SCB specimens with  
154 a single pre-existing crack were used. The setup allows the testing under  
155 mode I, mode II, and mixed-mode (I+II) loading conditions by simply varying  
156 the crack angles using the same specimen configuration and the same  
157 experimental set up [17]. The fracture toughness with different modes can be  
158 calculated from Eqs. 1-3 [10, 17]

$$159 \quad K_{ic} = \frac{P_i \sqrt{\pi a}}{2Rt} Y_i, \quad i=I, II \quad (1)$$

160 
$$K_E = \sqrt{K_{Ic}^2 + K_{IIc}^2} \quad (2)$$

161 
$$T = \frac{P_f}{2Rt} T^* \quad (3)$$

162 where:  $K_{Ic}$ ,  $K_{IIc}$  and  $K_E$  are mode I, mode II and mixed-mode fracture  
163 toughness, respectively (mixed-mode fracture toughness is also termed as  
164 effective fracture toughness (ETF) in the study.);  $T$  is the T-stress in SCB  
165 specimens;  $P_f$  is the peak load at the time of sample failure;  $a$  is the crack  
166 length;  $R$  denotes the sample radius and  $t$  represents the sample thickness.  $Y_I$   
167 and  $Y_{II}$  are dimensionless geometry factors for mode I and mode II loading  
168 conditions, respectively; and  $T^*$  also is a geometry factor and values of these  
169 factors of SCB specimens are depended on the crack length ( $a$ ), span length  
170 ( $2s$ ) as well as crack angle ( $\beta$ ).

171 The three-dimensional Particle Flow Code which implements the DEM  
172 technique was used to construct the SCB specimens. Particles having a  
173 radius ranging between 0.8 and 1.2 mm, which follows a uniform distribution,  
174 were used and a total of 22666 particles were generated (Fig. 2a). A loading  
175 bar (red, Fig. 2) was generated on the top of the SCB specimens and two  
176 supporting bars (blue) were created at the bottom with varying spans (i.e.,  $2s$ ).  
177 A constant loading rate (LR) of 0.001 m/s was applied on the loading bar to  
178 simulate static equilibrium state. Simulations terminated when the axial load  
179 ( $P$ ) dropped to 70 % of peak load, and the peak load was monitored and used  
180 for the calculation of fracture toughness based on Eqs. 1-3. In the  
181 construction of the DEM specimens, two different contact models were used  
182 to bond the particles (see the close-up view, Fig. 2a). The flat joint contact  
183 model (FJCM) was used for bonding the particles of the rock matrix to  
184 eliminate the intrinsic drawback of the standard bonded particle model [19, 20]  
185 (i.e., unrealistic low compressive-to-tensile strength ratio); while the smooth  
186 joint contact model (SJCM) was selected for bonding the particles laying on  
187 the opposite side of the bedding planes to eliminate unrealistic dilation arising  
188 from the spherical particles [21].

189 In the study, a total of 340 DEM specimens with different geometrical and  
190 geological properties were prepared. The specimen radius ( $R$ ) and thickness  
191 ( $t$ ) remained constant, which were 50 and 30 mm, respectively (Fig. 2). The  
192 crack length ( $a$ ) and span length ( $2s$ ) were varied within the range  
193 recommended by ISRM [17] (i.e.,  $0.4 \leq a/R \leq 0.6$  and  $0.5 \leq s/2R \leq 0.8$ ).  
194 Specifically, the crack length were 20, 25 and 30 mm, respectively. For  
195 specimens with a crack length of 20 mm, a span length of 50 and 55 mm were  
196 selected respectively to ensure that all tested specimens having this specific  
197 crack length (i.e., 20 mm) can provide a complete mode of fracture toughness  
198 (i.e., mode I, mode II and mixed-mode I+II) [22]. Similarly, for specimens with  
199 a crack length of 25 and 30 mm, a span length of 50, 55 and 61 mm were  
200 selected, respectively.

201 The selection of the crack angle ( $\beta$ ) followed the relationships between the  
202 geometry factors (i.e.,  $Y_I$  and  $Y_{II}$ ) and crack angle for various combinations of  
203  $a/R$  and  $s/R$ , which are shown in Fig. 3. The corresponding geometry factors  
204 of the SCB specimens used in the study are listed in Table 1 [22]. To study  
205 the effect of geological anisotropy on fracture behaviour, transversely isotropic  
206 bedding planes with three principal orientations with respect to the loading  
207 direction (i.e., arrester orientation, Fig. 2a; divider orientation, Fig. 2b; and  
208 short transverse orientation, Fig. 2c) were added into the specimens. The  
209 spacing of the bedding planes ( $d$ ) remained the constant, which was 17.5 mm  
210 [23].

### 211 **3.2 Calibration**

212 Calibration of the particulate DEM model in this study involved the selection of  
213 micro-parameters of SJCM and FJCM. As described earlier, an incipient  
214 bedding plane with a direct tensile strength of 1.82 MPa (87.5% intact parent  
215 rock strength) was mimicked in the study. The smooth joint properties  
216 corresponding to this bedding plane have been calibrated by Shang et al. [23]  
217 and are listed in Table 2. While in the calibration of FJCM, the procedure used  
218 by Shang et al. [19] was followed, in which uniaxial compressive tests were  
219 performed on medium-grained MGS specimens. Fig. 4a shows a  
220 representative axial stress-strain curve (black) and this curve was used for the

221 calibration of FJCM. A cylindrical DEM specimen with the same size (88 mm  
222 in length and 37 mm in diameter) as that used in the laboratory was  
223 generated. The DEM specimen was uniaxially compressed at a constant  
224 loading rate of 0.005 m/s through a trial-and-error process until the numerical  
225 results matched well with the experimental results. Fig. 4a shows a  
226 comparison of the representative stress-strain curves obtained in the  
227 laboratory test and DEM simulation. It can be seen that the simulated Young's  
228 modulus and peak strength agreed well with those measured from the  
229 laboratory experiment. The laboratory sample exhibited a clear shear failure  
230 pattern (Fig. 4b), which was however difficult to be reproduced in the DEM  
231 simulation (Fig. 4c). The main reason for the discrepancy between the  
232 simulated and experimental failure patterns is that the micro-cracks generated  
233 within the flat-jointed DEM model cannot coalesce easily and particle rotations  
234 were significantly suppressed due to the existence of the flat interfaces after  
235 bond failure [20], thus the split shear failure is difficult to be observed in the  
236 flat-jointed DEM model. Table 2 shows the corresponding calibrated micro-  
237 parameters. Apart from the above micro-parameters (need calibration), in the  
238 FJCM, some parameters are determined based on specific situations [19]. In  
239 this study, the flat-joint bonded and gapped fraction were set to 1 and 0,  
240 respectively, to assume that there were no initial micro-cracks in the DEM  
241 specimens. Minimum values of the radial and circumferential elements (1 and  
242 3, respectively) were used to reduce the calculation time [24].

243 To understand the failure characteristics of MGS under splitting, a numerical  
244 Brazilian tension test was additionally performed using the calibrated micro-  
245 parameters listed in Table 2. A Brazilian tensile strength of 2.7 MPa was  
246 simulated which matched well with experimental result (2.4 MPa [15]). The  
247 diametrical splitting failure pattern simulated in the Brazilian test agreed well  
248 with that observed in the laboratory (Fig. 5), although a compression-induced  
249 failure close to the top platen was also observed in the experiment (Fig. 5a).

## 250 **4. Numerical results**

### 251 **4.1 Axial load versus deflection**

252 Fig. 6 shows representative axial load-deflection plots ( $a/R=0.5$  and  
253  $s/R=0.55$ ), which are typical unimodal curves. The planar anisotropy (i.e.,  
254 bedding planes) were bedded in three principal orientations, as demonstrated  
255 by the insert diagrams (Figs. 6b-6d). Numerical results based on intact  
256 isotropic SCB specimens were included for comparison (Fig. 6a). The crack  
257 inclination angle,  $\beta$ , was varied from  $0^\circ$  to  $46^\circ$  for this case ( $a/R=0.5$  and  
258  $s/R=0.55$ ) to allow different modes of fracture toughness to be involved (i.e.,  
259 modes I and II and mixed-mode) [22].

260 As shown in Fig. 6, all axial loads were increased continuously until clear  
261 peak loads were reached; also for most curves, the peak loads increased with  
262 the increase of crack inclinations. The measured peak loads were used in the  
263 calculation of fracture toughness, which will be presented and discussed in  
264 Section 4.2. It was also observed that the curves within the pre-peak regions  
265 exhibited a quasi-linear behaviour, which is similar to the experimental  
266 observations in the fracture toughness tests on notched deep beam  
267 sandstones [25] and SCB Kimachi sandstones [9]. The non-linear behavior  
268 (cumulative deformation) observed in the laboratory experiments can be  
269 related to the compaction of micro-pores [26], as well as the pre-cut cracks  
270 [27] within the specimens used. The present study, however, hypothesize that  
271 the quasi-linear behavior observed in the pre-peak region in this DEM study  
272 was mainly due to the insignificant closure of the cracks, since there is wide  
273 acceptance of the fact that compaction of rock matrix or pores observed in the  
274 laboratory is extremely difficult to come by in the particle-based DEM  
275 simulations [19, 20, 23].

276 The post-peak curves in the study however exhibited three different  
277 responses. The first response consisted of a clear peak load and an abrupt  
278 load drop to the test end. This response appeared for all cases of intact MGS  
279 ( $\beta=0^\circ - 46^\circ$ , Fig. 6a) and few cases of horizontally bedded MGS (arrester) with  
280 relatively lower crack inclinations (e.g.,  $\beta=0^\circ$  and  $10^\circ$ , Fig. 6b). In literature,  
281 the abrupt failure response in fracture toughness experiments has been  
282 consistently observed [12, 25, 28], which is associated with the brittle nature  
283 of rocks. The second response also demonstrated a clear peak, followed  
284 however by significant load fluctuations until the complete failure of the

285 specimens (see  $\beta=35^\circ$  -  $46^\circ$  in Fig. 6b and  $\beta=0^\circ$  -  $30^\circ$  in Fig. 6c). The  
286 observed load fluctuation was related to the strength difference between the  
287 bedding planes and the rock matrix, leading to a complex load-deflection  
288 curve. In the third response mode, two load drops in the post-peak regions  
289 were observed (e.g.,  $\beta=45^\circ$ , Fig. 6d); and the first load drop following the peak  
290 load was much smaller than the second one. The load fluctuations observed  
291 in this response was due to the fact that the vertically orientated bedding  
292 planes with the same direction as that of the applied load significantly affected  
293 the integrity of the tested specimens. Particularly, the load-deflection  
294 response of the case  $\beta=10^\circ$  (Fig. 6d) exhibited more uncertainties, for which  
295 the bedding planes dominated the failure pattern, which will be examined  
296 further in Section 4.3.

#### 297 **4.2 Broad-spectrum peak loads and effective fracture toughness**

298 The effective fracture toughness (EFT) of MGS with a broad-spectrum  
299 magnitudes ranging between 0.1 and 0.6 MPa m<sup>1/2</sup> is shown in Fig. 7, where  
300 peak loads, in a wide range between 250 and 2000 N, are also included. The  
301 crack angles corresponding to mode II fracture toughness for each  
302 combination of  $s/R$  and  $a/R$  are marked blue in the figure.

303 The simulated peak loads increased gradually with the increase of crack  
304 inclinations, but with different extents which was mainly affected by crack  
305 length, as shown in Fig. 7. A wider range of peak loads (1.0-2.0 kN, Figs. 7g  
306 and 7h) was observed for DEM specimens with a smaller crack length  
307 ( $a/R=0.4$ ), in comparison with that (0.75-1.5 kN, see Figs. 7a-7c) measured by  
308 using the specimens with a larger crack length ( $a/R=0.6$ ). The EFT, however,  
309 decreased gradually for all cases when the crack inclination,  $\beta$ , was increased  
310 from  $0^\circ$  to a specific angle reflecting mode II fracture toughness. It can also be  
311 seen in Fig. 7 that the DEM specimens with short transverse planar  
312 anisotropy exhibited relatively smaller EFT (blue dots) compared with those  
313 values measured using the specimens with arrester and divider planar  
314 anisotropy (red and green dots, respectively). Similar observations have been  
315 reported for Mancos shale [3]; however, in their study only mode I fracture  
316 toughness was investigated. Additionally, a clear load drop was observed in

317 this study for the short transverse scenarios when the crack inclination  $\beta$  was  
318 increased from  $0^\circ$  to  $10^\circ$ . For example, as shown in Fig. 7e, the peak load  
319 measured under the mode I level ( $\beta=0^\circ$ ) was 0.75 kN, it was then decreased to  
320 around 0.43 kN when the crack inclination  $\beta$  was increased to  $5^\circ$ ; a further  
321 decrease (just below 0.35) was observed when  $\beta=10^\circ$ . After that the peak  
322 load was gradually increased with the increase in crack inclination. The peak  
323 load reduction described above was probably attributed to the deflection of  
324 induced fractures into weaker bedding planes, leading to a smaller peak load  
325 [4].

326 To further understand the effects of crack length ( $a/R$ ) and span length ( $s/R$ )  
327 on EFT, the broad range values of EFT (in Fig. 7) were plotted against mode I  
328 fracture toughness for different crack lengths (Fig. 8a) and span lengths (Fig.  
329 8b), without showing the effect of geological anisotropy. It can be seen that  
330 the EFT reported in this study was approximately linearly correlated with the  
331 mode I fracture toughness, irrespective of crack length and span length. More  
332 interestingly, somewhat larger values of EFT (0.4-0.6 MPa m<sup>1/2</sup>) were  
333 measured for specimens with relatively large crack length (i.e., 30 mm, sky  
334 blue dots in Fig. 8a); and fracture toughness of specimens with smaller cracks  
335 (20 mm) clustered within the range between 0.1 and 0.35 MPa m<sup>1/2</sup> (blue dots  
336 in Fig. 8a). This cluster phenomenon, however, was not observed in Fig. 8b,  
337 where span length was differentiated.

### 338 4.3 Failure characteristics

339 Representative failure characteristics of MGS specimens under mixed-mode  
340 loading are shown in Figs. 9-12, where  $s/R=0.5$  and  $a/R=0.55$ . Planar  
341 anisotropy was oriented in three principal orientations relative to the load  
342 direction and the crack inclination angle was varied between  $0^\circ$  and  $46^\circ$ . The  
343 failure patterns revealed in the DEM simulations were compared with  
344 experimental observations reported in literature. Fig. 9a shows the failure  
345 patterns of intact MGS specimens containing a crack with different  
346 inclinations. Tensile micro-cracks were marked red and shear micro-cracks  
347 were shown as black; and the macro-cracks were formed by the initiation and  
348 coalescence of the micro-cracks. Fracture initiation angle  $\theta_0$  was illustrated in

349 Fig. 9a (see  $\beta=40^\circ$ ). The numerical results in the study showed that the  
350 macro-cracks were induced between the tips of the pre-existing cracks and  
351 the loading points (see Fig. 9a); and all these macro-cracks were not planar in  
352 shape but showed some curvatures, which were quite similar in pattern to the  
353 experimental observations (Fig. 9b) [29]. Simulation results also revealed that  
354 the micro-mechanical failure of rock matrix/particles involved both tensile and  
355 shear micro-cracks (see the failure planes in Fig. 9a). This observation agreed  
356 with Backers et al. [30] and Backers and Stephansson [31], who argued that  
357 fracturing rock always involved a mixed mode pattern at micro-scale.

358 The failure patterns of MGS specimens containing arrester planar anisotropy  
359 are shown in Figs. 10a-10i. It can be seen that the induced macro-fractures  
360 were similar in shape to those generated within the intact MGS specimens  
361 (Fig. 9a), although some slight diversion of the fracture planes can be  
362 observed (see Figs. 10a, 10c and 10d). The observed diversion are attributed  
363 to the geological anisotropy, i.e., the arrester bedding planes affected the  
364 integrity of the DEM specimens. The slight diversion in fracture plane  
365 orientation was also observed by Lee et al. [11] in their investigation of  
366 fracture toughness of veined shale (see Fig. 10k). As it is anticipated that for  
367 SCB specimens with arrester planar anisotropy, the induced macro-cracks did  
368 not divert into the weakness planes, but were developed and passed through  
369 the anisotropic plane (Fig. 10i). This phenomenon was similarly observed in  
370 other geo-materials such as bedded coal (Fig. 10j) [32] and a Chinese  
371 sandstone (Fig. 10m) [27].

372 The failure patterns of MGS specimens containing divider planar anisotropy  
373 are presented in Fig. 11, in which it can be seen that the macro-fractures were  
374 similar in shape in comparison with those observed in Figs. 9 and 10. For the  
375 mode I case (Fig. 11,  $\beta=0^\circ$ ), the macro-fracture initiated at the tip of the pre-  
376 existing crack but propagated with relatively large diversion compared with  
377 that observed in Fig. 10a, leading to an irregular-shaped macro-fracture. The  
378 pure mode II fracture toughness was measured when  $\beta=46^\circ$  (Fig. 11); and a  
379 perfect curved failure plane was generated. As previously described, the  
380 mixed-mode fracture toughness was achieved by varying  $\beta$  from  $10^\circ$  to  $45^\circ$ ,  
381 as shown in Fig. 11. To allow a 3D observation of the internal structure, a top

382 view of a DEM specimen with  $\beta = 30^\circ$  (see Fig. 11 at the right corner) is  
383 presented, where particles are not shown for clarity. The bedding planes and  
384 the induced macro-fracture, as well as a thin section along the pre-existing  
385 crack are included. It clearly can be seen that the induced macro-fracture  
386 consisted of both tensile and shear micro-cracks (as discussed earlier); also  
387 the generated fracture crossed the bedding planes. It is important to note that  
388 although the failure patterns observed in Figs 9-11 only exhibited slight  
389 differences, such insignificant differences have led to a significant difference  
390 in the magnitude peak load, which was sensitive to the external conditions  
391 (Fig. 7).

392 As shown in Fig. 7 and discussed in Section 4.2, much smaller peak loads  
393 and EFT were measured for MGS specimens having short transverse planar  
394 anisotropy. Some typical failure patterns of MGS specimens with short  
395 transverse bedding planes are shown in Fig. 12. As can be seen in this figure,  
396 for the case  $\beta=0^\circ$ , the failure characteristic was very similar to that of intact  
397 rock (Fig. 9a,  $\beta=0^\circ$ ). While a significant diversion failure along an adjacent  
398 bedding plane was observed when  $\beta$  was increased up to  $10^\circ$  (see the close-  
399 up view in Fig. 12,  $\beta=10^\circ$ ). The diversion failure has led to a dramatic drop of  
400 peak load, as shown in Fig.7e (blue dots). However, no significant failures  
401 along the bedding planes were observed when  $\beta$  were further increased to  
402  $30^\circ$  and  $45^\circ$ ; instead, the macro-cracks passed through the planar anisotropy  
403 (Fig. 12,  $\beta=30^\circ$  and  $45^\circ$ ). It is important to note that this observed failure  
404 pattern was depended on the strength/inciency of bedding planes used in  
405 the study. A discussion in this regard will be offered in Section 6, during which  
406 bedding planes with a smaller tensile strength was examined. Another  
407 interesting observation was that the fracture initiation point for case  $\beta=45^\circ$   
408 (Fig. 12) was not exactly from the tip of the pre-existing crack but from the  
409 side which was slightly below the tip. This type of complex fracture  
410 propagation was also observed by Lee et al. [11].

411 To further understand the deformation of the MGS specimens under mixed-  
412 mode loading, an example of velocity distribution of particles is shown in Fig.  
413 13, with an emphasis of the areas close to the pre-existing cracks (shown in  
414 the close-up views). The particles are shown as arrows with directions. As can

415 be seen in Fig. 13a, the velocity of particles was not equally distributed; the  
416 particles around the pre-existing crack on the top section of the specimen  
417 exhibited a much smaller velocity ( $\sim 1.0e^{-3} \text{ ms}^{-1}$ ) compared with that of  
418 particles ( $\sim 1.0e^{-2} \text{ ms}^{-1}$ ) on the base of the specimen. As can be anticipated  
419 that the particles on the two sides of the pre-existing cracks moved in  
420 opposite directions, leading to the gradual opening of the pre-existing cracks,  
421 thereby the generation of the macro-fractures. For the specimens with  
422 bedding planes distributed in arrester (Fig. 13b) and divider (Fig. 13c)  
423 orientations, the velocity directions of the particles were affected by the  
424 orientations of the bedding planes and the magnitudes of the particle velocity  
425 of these two cases increased in general in comparison with that observed in  
426 Fig. 13a. For the case with the short transverse oriented beds (Fig. 13d), a  
427 larger range of particle velocity was observed for most of the particles (up to  
428  $3.2 e^{-2} \text{ ms}^{-1}$ , represented by yellow arrows), which probably can be attributed  
429 to the deformation of the short transverse bedding planes.

## 430 **5. Theoretical analysis of the mixed-mode fracture behaviour of MGS** 431 **and comparison study**

432 In literature, several fracture criteria have been proposed and used to predict  
433 mixed-mode fracture behaviour of solid materials [10, 33-36]. In this section,  
434 the mixed-mode fracture toughness of semi-circular MGS specimens was  
435 examined by using four different fracture criteria, which are based on stress  
436 and strain analysis, and the analysis of energy density. Specifically, the  
437 mixed-mode fracture toughness was expressed in the form of  $K_{Ic}/K_{Ec}$  (for  
438 comparison purpose) based on the criteria including generalized maximum  
439 tangential stress (GMTSS) criterion, conventional maximum tangential stress  
440 (CMTSS) criterion, generalized maximum tangential strain (GMTSN) criterion  
441 and generalized average strain energy density (GASED). The predictions of  
442 fracture initiation angle and effective fracture toughness required to validate  
443 the numerical results were reported.

### 444 **5.1 Prediction of mixed-mode fracture behaviour based on fracture** 445 **criteria**

446 5.1.1. Fracture behaviour predictions based on the GMTSS and CMTSS  
447 criteria

448 According to the Linear Elastic Fracture Mechanics (LEFM), the elastic  
449 tangential stress,  $\sigma_{\theta\theta}$ , in the vicinity of a crack tip subjected to mixed-mode  
450 loading can be written as [36]

$$451 \quad \sigma_{\theta\theta} = \frac{1}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left( K_{\text{I}} \cos^2 \frac{\theta}{2} - \frac{3}{2} K_{\text{II}} \sin \theta \right) + T \sin^2 \theta + O(r^{1/2}) \quad (4)$$

452 where  $r$  and  $\theta$  represent the polar coordinates with the origin at the crack tip.

453 In the GMTSS criterion, it is assumed that crack growth initiates radially from  
454 the crack tip along a specific direction of  $\theta_0$  (i.e., fracture initiation angle).

455 Crack extension takes place when the tangential stress  $\sigma_{\theta\theta}$  along  $\theta_0$  and at a  
456 critical distance  $r_c$  from the crack tip reaches a critical value  $\sigma_{\theta\theta c}$ . Both  $r_c$  and  
457  $\sigma_{\theta\theta c}$  are assumed to be material properties (i.e., they are constants for a  
458 specific solid material). It is noted that the CMTSS criterion only takes into

459 account the singular term (i.e.,  $\frac{1}{\sqrt{2\pi r}} \cos \frac{\theta}{2} (K_{\text{I}} \cos^2 \frac{\theta}{2} - \frac{3}{2} K_{\text{II}} \sin \theta)$ ) in Eq. (4)

460 [37]. However in the GMTSS criterion, the effect of  $T$ -stress is also considered  
461 in addition to the singular term.

462 According to the GMTSS criterion, one can obtain

$$463 \quad \left. \frac{\partial \sigma_{\theta\theta}}{\partial \theta} \right|_{\theta=\theta_0} = 0 \quad (5)$$

464 Thus, the fracture initiation angle  $\theta_0$  under mixed-mode loading is determined  
465 from

$$466 \quad [K_{\text{I}} \sin \theta_0 + K_{\text{II}} (3 \cos \theta_0 - 1)] - \frac{16T}{3} \sqrt{2\pi r_c} \cos \theta_0 \sin \frac{\theta_0}{2} = 0 \quad (6)$$

467 As described earlier, the brittle fracture takes place when

$$468 \quad \sigma_{\theta\theta}(r_c, \theta_0) = \sigma_{\theta\theta c} \quad (7)$$

469 By replacing the angle  $\theta_0$  from Eq. (6) into Eq. (7), the fracture is predicted to  
470 initiate when

471 
$$\sqrt{2\pi r_c} \sigma_{\theta\theta c} = \cos \frac{\theta_0}{2} (K_I \cos^2 \frac{\theta_0}{2} - \frac{3}{2} K_{II} \sin \theta_0) + \sqrt{2\pi r_c} T \sin^2 \theta \quad (8)$$

472 To further study the fracture initiation angle and onset fracture, two biaxiality  
473 ratio,  $B$  and  $\alpha$ , are defined as follows [36, 37]:

474 
$$B = T\sqrt{\pi a} / K_E \quad (9)$$

475 
$$\alpha = \sqrt{\frac{2r_c}{a}} \quad (10)$$

476 It is noted that  $B$  is geometry factor and its values for SCB specimens with  
477 different  $a/R$  and  $s/R$  have been deduced by Ayatollahi and Aliha [22] and are  
478 shown in Table 1.

479 Eq. (8) can be rewritten in terms of  $B\alpha$  and  $K_{Ic}$

480 
$$K_{Ic} = \cos \frac{\theta_0}{2} (K_I \cos^2 \frac{\theta_0}{2} - \frac{3}{2} K_{II} \sin \theta_0) + B\alpha K_E \sin^2 \theta_0 \quad (11)$$

481 Thus, one can get

482 
$$\frac{K_{Ic}}{K_E} = \frac{1}{K_E} [\cos \frac{\theta_0}{2} (K_I \cos^2 \frac{\theta_0}{2} - \frac{3}{2} K_{II} \sin \theta_0)] + B\alpha \sin^2 \theta_0 \quad (12)$$

483 Replacing Eqs. (1), (2), (9), (10) into Eq. (12), the relationship between  $K_{Ic}$   
484 and  $K_E$  can be rewritten in terms of geometry factors  $Y_I$ ,  $Y_{II}$ , and  $T^*$  as

485 
$$\frac{K_{Ic}}{K_E} = \frac{1}{\sqrt{Y_I^2 + Y_{II}^2}} [\cos \frac{\theta_0}{2} (Y_I \cos^2 \frac{\theta_0}{2} - \frac{3}{2} Y_{II} \sin \theta_0) + T^* \sqrt{\frac{2r_c}{a}} \sin^2 \theta_0] \quad (13)$$

486 Similarly, substituting Eqs. (1) and (3) into Eq. (6), the fracture initiation angle  
487  $\theta_0$  under mixed-mode loading can be rewritten in terms of geometry factors  $Y_I$ ,  
488  $Y_{II}$ , and  $T^*$  as

489 
$$Y_I \sin \theta_0 + Y_{II} (3 \cos \theta_0 - 1) - \frac{16T^*}{3} \sqrt{\frac{2r_c}{a}} \cos \theta_0 \sin \frac{\theta_0}{2} = 0 \quad (14)$$

490 Thereby the Eqs. (13) and (14) can be used to predict the mixed-mode  
491 effective fracture toughness  $K_E$  and the fracture initiation angle  $\theta_0$ ,

492 respectively. The CMTSS criterion can be obtained when  $T^*$  in the Eqs. (13)  
 493 and (14) are ignored (i.e.,  $T^*=0$ ).

#### 494 5.1.2. Fracture behaviour prediction based on the GMTSN criterion

495 It is also known that the elastic radial stress,  $\sigma_{rr}$ , in the vicinity of a crack tip  
 496 subjected to mixed-mode loading can be written as [36]

$$497 \quad \sigma_{rr} = \frac{1}{\sqrt{2\pi r}} \cos \frac{\theta}{2} [K_I(1 + \sin^2 \frac{\theta}{2}) + K_{II}(\frac{3}{2} \sin \theta - 2 \tan \frac{\theta}{2})] + T \cos^2 \theta + O(r^{1/2}) \quad (15)$$

498 According to the Hooke's Law and combining Eqs. (4) and (15), the tangential  
 499 strain,  $\varepsilon_{\theta\theta}$ , in the vicinity of the crack can be written as

$$500 \quad \varepsilon_{\theta\theta} = \frac{1+\nu}{E} [k\sigma_{\theta\theta} + (k-1)\sigma_{rr}] = \frac{1+\nu}{E\sqrt{2\pi r}} [K_I f_1(\theta) + K_{II} f_2(\theta) + T\sqrt{2\pi r} f_3(\theta)] \quad (16)$$

501 where  $k = 1/(1+\nu)$  represents plane stress condition and  $k = (1-\nu)$  stands  
 502 for plane strain condition;  $E$  and  $\nu$  are the Young's modulus and Poisson's

503 ratio, respectively.  $f_1(\theta) = \frac{1}{4} [(8k-5) \cos \frac{\theta}{2} + \cos \frac{3\theta}{2}]$ ,

504  $f_2(\theta) = -\frac{1}{4} [(8k-5) \sin \frac{\theta}{2} + 3 \sin \frac{3\theta}{2}]$  and  $f_3(\theta) = k - \cos^2 \theta$ .

505 According to the GMTSN criterion, crack growth initiates radially from the  
 506 crack tip along the direction of  $\theta_0$ ; and crack extension takes place when the  
 507 tangential strain  $\varepsilon_{\theta\theta}$  along  $\theta_0$  and at a critical distance  $r_c$  from the crack tip  
 508 attains a critical value  $\varepsilon_{\theta\theta c}$ . Both  $r_c$  and  $\varepsilon_{\theta\theta c}$  are assumed to be material  
 509 properties. The GMTSN criterion can be expressed as

$$510 \quad \begin{cases} \left. \frac{\partial \varepsilon_{\theta\theta}}{\partial \theta} \right|_{\theta=\theta_0} = 0 \\ \varepsilon_{\theta\theta}(r_c, \theta_0) = \varepsilon_{\theta\theta c} \\ \left. \frac{\partial^2 \varepsilon_{\theta\theta}}{\partial \theta^2} \right|_{\theta=\theta_0} < 0 \end{cases} \quad (17)$$

511 Replacing Eq. (16) into Eq. (17), the fracture initiation angle  $\theta_0$  in terms of  
 512 geometry factors ( $Y_I$  and  $Y_{II}$ ) can be written as

513 
$$Y_I[(5-8k)\sin\frac{\theta_0}{2}-3\sin\frac{3\theta_0}{2}]+Y_{II}[(5-8k)\cos\frac{\theta_0}{2}-9\cos\frac{3\theta_0}{2}]$$
 (18)

514 
$$+8B\alpha\sqrt{Y_I^2+Y_{II}^2}\sin 2\theta_0=0$$

514 Substituting the fracture initiation angle  $\theta_0$  (obtained from Eq. 18) and Eqs. (2)

515 (9) and (10) into Eq. (16), one can obtain

516 
$$\varepsilon_{\theta_0\theta_0}E\sqrt{2\pi r_c}=(1+\nu)[K_I f_1(\theta_0)+K_{II} f_2(\theta_0)+B\alpha K_E f_3(\theta_0)]$$
 (19)

517 For the conventional mode I loading condition,  $K_I=K_{Ic}$ ,  $K_{II}=0$  and  $\theta_0=0$ , the

518 following equation can be obtained according to Eqs. (17) and (19).

519 
$$\varepsilon_{\theta_0\theta_0}E\sqrt{2\pi r_c}=(1+\nu)[(2k-1)+B\alpha(k-1)]K_{Ic}, (B\alpha-\frac{(2k-1)}{8}<0)$$
 (20)

520 Combining Eqs. (19) and (20), one can obtain

521 
$$\frac{K_I f_1(\theta_0)+K_{II} f_2(\theta_0)+B\alpha K_E f_3(\theta_0)}{[(2k-1)+B\alpha(k-1)]K_{Ic}}, (B\alpha-\frac{(2k-1)}{8}<0)$$
 (21)

522 Dividing both sides of Eq. (21) by  $K_E$ , the mixed-mode fracture (in the form of

523  $\frac{K_{Ic}}{K_E}$ ) can be predicted and written in terms of geometry factors ( $Y_I$  and  $Y_{II}$ ) as

524 
$$\frac{K_{Ic}}{K_E}=\frac{(\frac{Y_I f_1+Y_{II} f_2}{\sqrt{Y_I^2+Y_{II}^2}})+B\alpha f_3}{(2k-1)+B\alpha(k-1)}, (B\alpha-\frac{(2k-1)}{8}<0)$$
 (22)

### 525 5.1.3. Fracture behaviour prediction based on the GASED criterion

526 For the plane elasticity problems, the strain energy density function,  $dW/dV$ ,

527 stored in an element can be written as [38]

528 
$$dW/dV=\frac{1}{2G}[\frac{m+1}{8}(\sigma_{rr}+\sigma_{\theta\theta})^2-\sigma_{rr}\sigma_{\theta\theta}+\sigma_{r\theta}^2]$$
 (23)

529 where  $G$  is the modulus of rigidity and it is known that  $G=E/2(1+\nu)$ .  $m$  is an

530 elastic constant and  $m=3-4\nu$ ,  $m=\frac{3-\nu}{1+\nu}$  for plane strain and plane stress

531 problems, respectively.

532 According to Smith et al. [36] and the Airy stress function proposed by  
 533 Williams [39], the stress  $\sigma_{r\theta}$  in the vicinity of a crack tip subjected to mixed-  
 534 mode loading can be written as

$$535 \quad \sigma_{r\theta} = \frac{1}{2\sqrt{2\pi r}} \cos \frac{\theta}{2} [K_I \sin \frac{\theta}{2} + K_{II} (3 \cos \theta - 1)] - T \sin \theta \cos \theta + O(r^{1/2}) \quad (24)$$

536 The average strain energy density factor  $S$ , reflecting the strength of the  
 537 elastic energy field in the vicinity of the crack tip, is defined as [38]

$$538 \quad S = r dW/dV \quad (25)$$

539 Substituting the stress components from Eqs. (4), (15), (23) and (24) into Eq.  
 540 (25), the following can be derived

$$541 \quad S = A_1 K_I^2 + A_2 K_{II}^2 + 2A_3 K_I K_{II} + 2A_4 T K_I \sqrt{2\pi r} + 2A_5 T K_{II} \sqrt{2\pi r} + A_6 2\pi r T^2 \quad (26)$$

542 where

$$543 \quad \left\{ \begin{array}{l} A_1 = \frac{1}{16\pi G} [(m - \cos \theta)(1 + \cos \theta)] \\ A_2 = \frac{1}{16\pi G} [m(1 - \cos \theta) + \cos \theta(1 + 3 \cos \theta)] \\ A_3 = \frac{1}{16\pi G} \sin \theta (2 \cos \theta - m + 1) \\ A_4 = \frac{1}{16\pi G} \cos \frac{\theta}{2} (\cos 2\theta - \cos \theta + m - 1) \\ A_5 = -\frac{1}{16\pi G} \sin \frac{\theta}{2} (\cos 2\theta + \cos \theta + m + 1) \\ A_6 = \frac{1}{16\pi G} \left(\frac{m+1}{2}\right) \end{array} \right. \quad (27)$$

544 According to the GASED criterion, crack growth initiates radially from the  
 545 crack tip along the direction of  $\theta_0$  where the amount of the strain energy  
 546 density factor is minimum at a critical distance  $r_c$  from the crack tip. The  
 547 GASED criterion can be expressed as

$$548 \quad \left. \frac{\partial S}{\partial \theta} \right|_{\theta=\theta_0} = 0 \quad (28)$$

549 Thus the fracture initiation angle  $\theta_0$  can be determined and written in terms of  
 550 the geometry factors ( $Y_I$  and  $Y_{II}$ ) using the following equations

$$551 \quad C_1 Y_I^2 + C_2 Y_{II}^2 + C_3 Y_I Y_{II} + C_4 B\alpha Y_I \sqrt{Y_I^2 + Y_{II}^2} \\ + C_5 B\alpha Y_{II} \sqrt{Y_I^2 + Y_{II}^2} + C_6 (B\alpha)^2 (Y_I^2 + Y_{II}^2)^2 = 0 \quad (29)$$

552 where

$$553 \quad \left\{ \begin{array}{l} C_1 = \frac{1}{16\pi G} \sin \theta_0 (2 \cos \theta_0 - m + 1) \\ C_2 = -\frac{1}{16\pi G} \sin \theta_0 (6 \cos \theta_0 - m + 1) \\ C_3 = \frac{1}{8\pi G} (2 \cos 2\theta_0 - m \cos \theta_0 + \cos \theta_0) \\ C_4 = -\frac{1}{16\pi G} \sin \frac{\theta_0}{2} (5 \cos 2\theta_0 + \cos \theta_0) + m + 1 \\ C_5 = -\frac{1}{16\pi G} \cos \frac{\theta_0}{2} (5 \cos 2\theta_0 - \cos \theta_0) + m + 3 \\ C_6 = 0 \end{array} \right. \quad (30)$$

554 According to the GASED criterion, fracture takes place when  $S$  reaches its  
 555 critical value  $S_c$

$$556 \quad S = S_c \quad (31)$$

557 Substituting the fracture initiation angle  $\theta_0$  (obtained from Eq. 29) and Eqs.  
 558 (2), (9), (10) and (26) into Eq. (31), the fracture can be predicted by

$$559 \quad S_c = A_1 K_I^2 + A_2 K_{II}^2 + A_3 K_I K_{II} + A_4 B\alpha K_E K_I \\ + A_5 B\alpha K_E K_{II} + A_6 (B\alpha K_E)^2 \quad (32)$$

560  $S_c$  is a constant material property and as described by Sih [35], this property  
 561 can be expressed by

$$562 \quad S_c = \frac{1}{8\pi G} (m-1) K_{Ic}^2 \quad (33)$$

563 Thus

$$564 \quad \frac{1}{8\pi G} (m-1) K_{Ic}^2 = A_1 K_I^2 + A_2 K_{II}^2 + A_3 K_I K_{II} + A_4 B\alpha K_E K_I \\ + A_5 B\alpha K_E K_{II} + A_6 (B\alpha K_E)^2 \quad (34)$$

565 Dividing both sides of Eq. (34) by  $K_E^2$ , the mixed-mode fracture (in the form of  
 566  $\frac{K_{Ic}}{K_E}$ ) can be predicted and written in terms of geometry factors ( $Y_I$  and  $Y_{II}$ ) as

$$\begin{aligned}
 & A_1 \left( \frac{K_{Ic}}{K_E} \right)^2 + A_4 B \alpha \frac{K_{Ic}}{K_E} - A_1 \left( \frac{Y_I}{\sqrt{Y_I^2 + Y_{II}^2}} \right)^2 \\
 567 & - A_2 \left( \frac{Y_{II}}{\sqrt{Y_I^2 + Y_{II}^2}} \right)^2 - A_3 \frac{Y_I Y_{II}}{Y_I^2 + Y_{II}^2} \quad (35) \\
 & - A_4 \frac{B \alpha Y_I}{\sqrt{Y_I^2 + Y_{II}^2}} - A_5 \frac{B \alpha Y_{II}}{\sqrt{Y_I^2 + Y_{II}^2}} = 0
 \end{aligned}$$

## 568 **5.2 Comparing the theoretical predictions of mixed-mode fracture** 569 **behaviour with that from DEM simulations**

570 Figs.14-16 show the inferred fracture initiation angle and EFT (in the form of  
 571  $K_E/K_{Ic}$ ) for different combinations of  $a/R$  (0.4, 0.5 and 0.6) and  $s/R$  (0.5, 0.55  
 572 and 0.61). For comparison, the previously reported DEM results are included  
 573 in those figures and shown as scattered dots. As shown in Fig.14 ( $a/R=0.4$ ;  
 574  $s/R=0.5$  and 0.55, respectively), the DEM simulation results in terms of  
 575 fracture initiation angle (Figs. 14a and 14c) and EFT (Figs. 14b and 14d)  
 576 agreed in broad with the predictions by the GMTSS, GMTSN and GASED  
 577 criteria. Nevertheless, slightly larger discrepancies between the theoretical  
 578 and numerical predictions still can be observed when the crack angle was  
 579 between  $20^\circ$  and  $35^\circ$  for the case  $a/R=0.4$  and  $s/R=0.5$  (Fig. 14b), as well as  
 580 when the crack angle was larger than  $50^\circ$  for the case  $a/R=0.4$  and  $s/R=0.55$   
 581 (Fig. 14d). Almost without exception, the CMTSS criterion overestimated EFT  
 582 and underestimated the fracture initiation angle.

583 A relatively large degree of discrepancy between the theoretical predictions  
 584 and the numerical results can be observed when  $a/R$  was increased to 0.5  
 585 (Fig.15), especially when  $s/R=0.55$ . For example, as can be seen in Figs. 15b,  
 586 15d and 15f, the DEM predicted  $K_E/K_{Ic}$  (scattered dots) for the specimens with  
 587 different orientations of planar anisotropy almost lay between the predictions  
 588 by the GMTSS criterion and the CMTSS criterion. This observation indicated  
 589 that the influence of geological anisotropy on fracture behaviour of the SCB  
 590 specimens used in the study became larger when the crack length  $a$  was

591 increased to the half of the specimen diameter  $R$ . It also can be seen that, for  
592 specimens with short transverse planar anisotropy, three unexpected values  
593 of  $K_E/K_{Ic}$  were numerically obtained (between 0.5 and 0.7) when crack angles  
594 were  $5^\circ$ ,  $10^\circ$  and  $15^\circ$ , respectively (Fig. 15d), which were much lower than the  
595 theoretical predictions (0.83-0.98).

596 As shown in Fig. 16, a better match between the simulated fracture behaviour  
597 and theoretical predictions can be seen when  $a/R$  was increased further to  
598 0.6, where  $s/R$  was varied from 0.5 to 0.61. Again, the CMTSS criterion  
599 exhibited poor performance in the prediction of fracture behaviour compared  
600 with the other three criteria (i.e., GMTSS, GMTSN and GASED criteria).

## 601 **6. Discussion**

602 The fracture toughness of rock materials can be measured in the laboratory  
603 using the specimens recommended by ISRM (i.e, SCB, SR and CBD  
604 specimens). The reliability of the laboratory-scale measurements however can  
605 be affected by many factors including geological anisotropy [3], geometrical  
606 properties of the specimens used [6], as well as experimental setup [17]. This  
607 fact is widely acknowledged, however it still lacks a systematic study on how  
608 these factors affect the fracture behaviour of anisotropic rocks. As such, in  
609 this study a comprehensive numerical analysis of the fracture behaviour of  
610 MGS was conducted and a broad-spectrum mixed-mode fracture toughness  
611 of this lithology was reported based on a total of 340 DEM simulations. The  
612 influences of planar anisotropy orientation, length and angle of the pre-  
613 existing cracks, as well as span length were considered in the DEM  
614 simulation. The DEM results were compared quantitatively with theoretical  
615 predictions and qualitatively with previous experimental observations.

616 Although a broad agreement has been observed in the comparison study  
617 (Figs. 14-17), some discrepancies still existed, especially for the cases when  
618  $a/R=0.5$  (Figs. 15b, 15d and 15f). The observed discrepancies can probably  
619 be related to: (1) the ignorance of the influence of geological anisotropy on the  
620 fracture behaviour of solid materials by the current fracture criteria [34, 36,  
621 38]; and (2) the inherent limitations of the DEM code used in the study (for  
622 example, the spherical assemblies were used in the present simulation to

623 represent real rock matrix, which is an assumption) [20, 21]. The frustrating  
624 performance of the CMTSS criterion in the prediction of fracture behaviour  
625 was also noted in this study, which is mainly due to the ignorance of the non-  
626 singular term in that criterion (i.e., the  $T$ -stress shown in Eqs. 13 and 14) [37].

627 Additionally, a diversion failure of fracture from rock matrix to pre-existing  
628 bedding planes was observed for short transverse bedded specimens with a  
629 relatively small crack inclination angle (i.e.,  $\beta < 15^\circ$ ), which has led to a distinct  
630 peak load drop (Fig. 7, blue dots). However, the diversion failure was not  
631 observed for arrester and divider bedded specimens, as well as for short  
632 transverse bedded specimens with a relatively high crack inclination angle  
633 (i.e.,  $\beta > 15^\circ$ ). It is important to note that the bedding planes with a tensile  
634 strength of 87.5 % that of parent rock was modelled in the study, thus the  
635 above failure observation only applies to the anisotropic rocks with relatively  
636 high tensile strength bedding planes/planar anisotropy.

637 Additional DEM fracture toughness simulations based on the SCB specimens  
638 ( $a/R=0.5$  and  $s/R=0.55$ ) containing short transverse bedding planes with a  
639 relatively low tensile strength (i.e., bedding planes with a tensile strength of  
640 31.3 % that of parent rock were used [23, 40] ). The corresponding micro-  
641 parameters of the low-strength bedding plane within MGS has been reported  
642 by Shang et al. [23] and are listed in Table 2. The numerical scheme is the  
643 same as that described in Section 3.1. The relationship between the axial load  
644 and deflection of the four additional simulations is shown in Fig. 17, with the  
645 simulated failure patterns (Figs. 17b-17e) and corresponding experimental  
646 observations included (Figs. 17f-17h) (The experiment was reported by Roy et  
647 al. [14]). It can be seen that the peak load increased with the increasing of the  
648 crack inclination angles ( $\beta$  from  $0^\circ$  to  $46^\circ$ , Fig. 17a). As expected, one planar  
649 failure plane was generated within the rock matrix when  $\beta=0^\circ$  (Fig.17b),  
650 which was very close to the observed patterns shown in Fig.12 ( $\beta=0^\circ$ ). At  
651  $\beta=20^\circ$  (Fig.17c), a non-planar failure plane was induced, with a combination  
652 failure of the adjacent bedding plane (the failure of bedding planes was  
653 represented by the pure tensile micro-cracks shown in red) and the rock  
654 matrix close to the loading point. This failure pattern was close to that shown  
655 in Fig. 17h, in which the cement joint planes with a similar tensile strength to

656 that of our weak bedding planes were used in the laboratory [14]. Notably, “Z”-  
657 shaped failure planes were observed when  $\beta$  were increased up to 30° (Fig.  
658 17d) and 46° (Fig.17e), respectively. In these two cases, fractures initiated at  
659 the pre-existing crack tips, and then propagated within the rock material  
660 before reaching the adjacent bedding planes. The pure tensile failures of the  
661 bedding planes were then observed (red micro-cracks in Figs.17d and 17e),  
662 followed by the failures of the rock materials close to the loading points.  
663 Similar observations were achieved by Roy et al. [14] in the laboratory (see  
664 Figs. 17f and 17g). It should be noted that the origin of the “Z”-shaped failure  
665 pattern observed in the study was largely dependent on the relative tensile  
666 strength of the planar anisotropy to that of the parent rock.

## 667 **7. Conclusions**

668 In this paper, a broad-spectrum mixed-mode fracture behaviour of an  
669 anisotropic sandstone was reported based on a 3D DEM study, where the  
670 ISRM-suggested SCB specimens with different geological and geometrical  
671 conditions (i.e., a combination of  $a/R$ ,  $s/R$ ,  $\beta$  and orientation of planar  
672 anisotropy) were used. The numerical findings of the study were validated  
673 against experimental observations and theoretical predictions and a good  
674 agreement was observed. Results of the study allow a new insight into the  
675 possible variations of the fracture toughness of anisotropic rocks (arising from  
676 the factors mentioned above). The main conclusions of this study are shown  
677 as follows:

678 (1) The axial load-deflection curves obtained in this numerical study exhibited  
679 three different responses in the post-peak region: 1) one abrupt load drop (for  
680 all specimens without planar anisotropy and few specimens with arrester  
681 oriented planar anisotropy); 2) significant load fluctuations until the complete  
682 failure of specimens (for most specimens with arrester and divider oriented  
683 planar anisotropy); and 3) two load drops (for most specimens with short  
684 transverse oriented planar anisotropy).

685 (2) A broad-spectrum effective fracture toughness (EFT) of Midgley Grit  
686 sandstone was revealed, which were between 0.1 and 0.6 MPa m<sup>1/2</sup>. The  
687 DEM specimens with short transverse planar anisotropy exhibited relatively

688 small EFT in comparison with those measured using the specimens with  
689 arrester and divider planer anisotropy. Furthermore, a distinct drop of EFT  
690 was observed in this study for the short transverse bedded specimens when  
691 the crack inclination  $\beta$  was increased from  $0^\circ$  to  $10^\circ$ .

692 (3) It was also concluded that the EFT of Midgley Grit sandstone was  
693 approximately linearly correlated with the mode I fracture toughness,  
694 irrespective of geological and geometrical conditions. Also, somewhat larger  
695 values of EFT ( $0.4\text{-}0.6 \text{ MPa m}^{1/2}$ ) were measured for the specimens with  
696 relatively large crack length (i.e., 30 mm in the study), in comparison with  
697 those values ( $0.1\text{-}0.35 \text{ MPa m}^{1/2}$ ) measured using the specimens with smaller  
698 crack length (20 mm in the study). The effect of span length on the magnitude  
699 of EFT was not significant.

700 (4) For the SCB specimens with a higher tensile strength planar anisotropy  
701 (1.82 MPa), the failure characteristics of the specimens in this study exhibited  
702 a similar pattern. The non-planar macro-fractures induced in the DEM  
703 specimens passed through the anisotropic planes, except for a few  
704 specimens containing short transverse planar anisotropy with a relatively low  
705 crack inclination angle ( $\beta < 10^\circ$ ), for which the diversion failure from the rock  
706 matrix to the weak planar anisotropy was observed. For specimens with a  
707 lower tensile strength anisotropic plane (0.65 MPa in the study), a much more  
708 complex failure pattern was observed for specimens containing short  
709 transverse planar anisotropy. A complex combination failure of rock matrix  
710 and planar anisotropy was observed, leading to a "Z"-shaped failure plane.

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832 **Fig Captions:**

833 **Fig. 1** Location (a) and (b) and simplified geological map (c) of the Blackhill  
834 Quarry (UK), where the anisotropic Midgley Grit sandstone (d) is mined. (e) A  
835 photomicrograph of thin section showing the mineralogy of the Midgley Grit  
836 sandstone.

837 **Fig. 2** Numerical setup of semi-circular bend MGS specimens with three  
838 principal orientations of planar anisotropy: (a) arrester; (b) divider and (c)  
839 short transverse. Close-up of flat joint and flat joint contacts is shown in (a).  
840 See text for more details about the geometrical parameters.

841 **Fig. 3** Geometry factors ( $Y_I$ ,  $Y_{II}$ ,  $T^*$  and  $B$ ) for SCB specimens with various  
842 combinations of  $s/R$  and  $a/R$ . The crack inclinations corresponding to the  
843 mode II fracture toughness for each combination are marked in red. (Adapted  
844 from [22])

845 **Fig. 4** (a) Comparison of unconfined stress-strain curves of MGS from  
846 laboratory test and DEM simulation; (b) failure pattern of an intact MGS after a  
847 uniaxial compression test; and (c) failure pattern of a DEM specimen  
848 uniaxially compressed.

849 **Fig. 5** Comparison of the failure patterns of Brazilian tests: (a) laboratory test  
850 and (b) DEM simulation.

851 **Fig. 6** Representative axial load-deflection curves of SCB specimens under  
852 mixed-mode loading ( $a/R=0.5$  and  $s/R=0.55$ ). (a) Intact MGS specimens  
853 without planar anisotropy and MGS specimens containing planar anisotropy  
854 with three principal orientations: (b) arrester, (c) divider and (d) short  
855 transverse.

856 **Fig. 7** Broad-spectrum peak loads and effective fracture toughness of  
857 anisotropic semi-circular MGS specimens with various combinations of  $a/R$ ,  
858  $s/R$  and  $\beta$ .

859 **Fig. 8** Effective fracture toughness against mode I fracture toughness for  
860 different crack lengths (a) and span lengths (b).

861 **Fig. 9** Failure patterns of SCB sandstone specimens without planar  
862 anisotropy: (a) DEM simulations of MGS and (b) laboratory tests on a Chinese  
863 sandstone [29]. The fracture initiation angle  $\theta_0$  is illustrated on the failed DEM  
864 specimen at  $\beta=40^\circ$ .

865 **Fig. 10** (a) Failure characteristics of semi-circular MGS specimens containing  
866 arrester planar anisotropy and crack inclination was varied from  $0^\circ$  (a) to  $46^\circ$   
867 (h) in the DEM simulations. A 3D view showing the arrester bedded planar  
868 anisotropy and the induced fracture was presented without showing the  
869 particles (i). Failure patterns of three different geo-materials with arrester  
870 planar anisotropy were included for comparison: (j) bedded coal [24]; (k)  
871 veined shale [11] and (m) a bedded Chinese sandstone [27].

872 **Fig. 11** Failure characteristics of semi-circular MGS specimens containing  
873 divider planar anisotropy. A 3D top view of the failed specimen with  $\beta =30^\circ$  is  
874 presented without showing the particles.

875 **Fig. 12** Typical failure patterns of MGS specimens with short transverse  
876 planar anisotropy.

877 **Fig. 13** An illustration of particle velocity (at micro-scale) of semi-circular MGS  
878 specimens under mixed-mode loading: (a) a cracked specimen without planar

879 anisotropy ( $\beta=30^\circ$ ); cracked specimens with arrester (b), divider (c) and short  
880 transverse (d) planar anisotropy. The particles are shown as arrows with  
881 orientations.

882 **Fig. 14** Comparison of the numerical results and theoretical predictions:  
883 Fracture initiation angle versus crack angle for (a)  $a/R=0.4$ ,  $s/R=0.5$  and (c)  
884  $a/R=0.4$ ,  $s/R=0.55$ ; and effective fracture toughness (in the form of  $K_E/K_{Ic}$ )  
885 against crack angle for (b)  $a/R=0.4$ ,  $s/R=0.5$  and (d)  $a/R=0.4$ ,  $s/R=0.55$ .

886 **Fig. 15** Comparison of numerical results and theoretical predictions: Fracture  
887 initiation angle versus crack angle for (a)  $a/R=0.5$ ,  $s/R=0.5$ ; (c)  $a/R=0.5$ ,  
888  $s/R=0.55$ ; and (e)  $a/R=0.5$ ,  $s/R=0.61$ ; as well as effective fracture toughness  
889 (in the form of  $K_E/K_{Ic}$ ) against crack angle for (b)  $a/R=0.5$ ,  $s/R=0.5$ ; (d)  
890  $a/R=0.5$ ,  $s/R=0.55$ ; and (f)  $a/R=0.5$ ,  $s/R=0.61$ .

891 **Fig. 16** Comparison of numerical results and theoretical predictions: Fracture  
892 initiation angle versus crack angle for (a)  $a/R=0.6$ ,  $s/R=0.5$ ; (c)  $a/R=0.6$ ,  
893  $s/R=0.55$ ; and (e)  $a/R=0.6$ ,  $s/R=0.61$ ; as well as effective fracture toughness  
894 (in the form of  $K_E/K_{Ic}$ ) against crack angle for (b)  $a/R=0.6$ ,  $s/R=0.5$ ; (d)  
895  $a/R=0.6$ ,  $s/R=0.55$ ; and (f)  $a/R=0.6$ ,  $s/R=0.61$ .

896 **Fig. 17** (a) Axial load versus deflection of four MGS specimens with weaker  
897 short transverse planar anisotropy (i.e., the bedding planes with a direct  
898 tensile strength of 31.3 % that of the parent rock). (b) - (d) Failure patterns of  
899 the four additional simulations and (f)-(h) similar failure patterns observed by  
900 Roy et al. [14] in their laboratory experiments.

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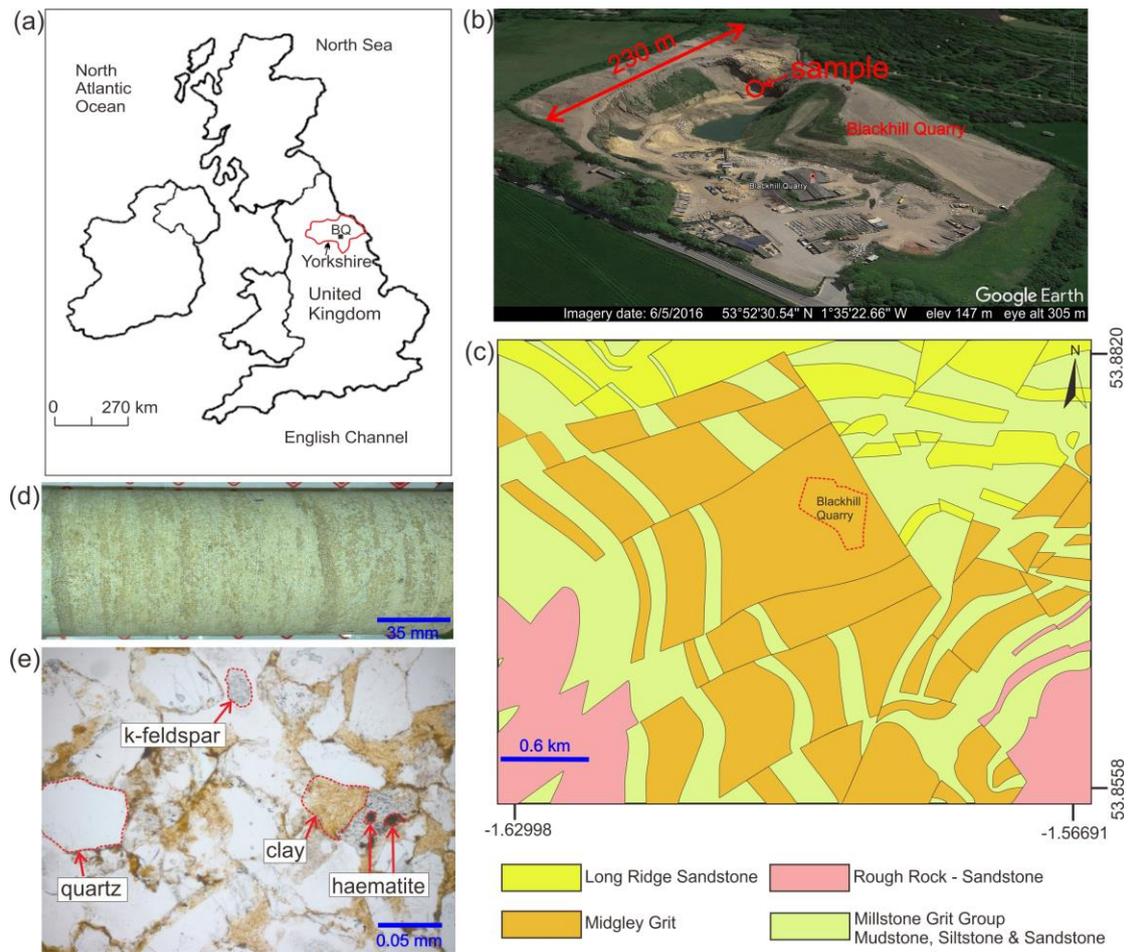
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**Fig 1**

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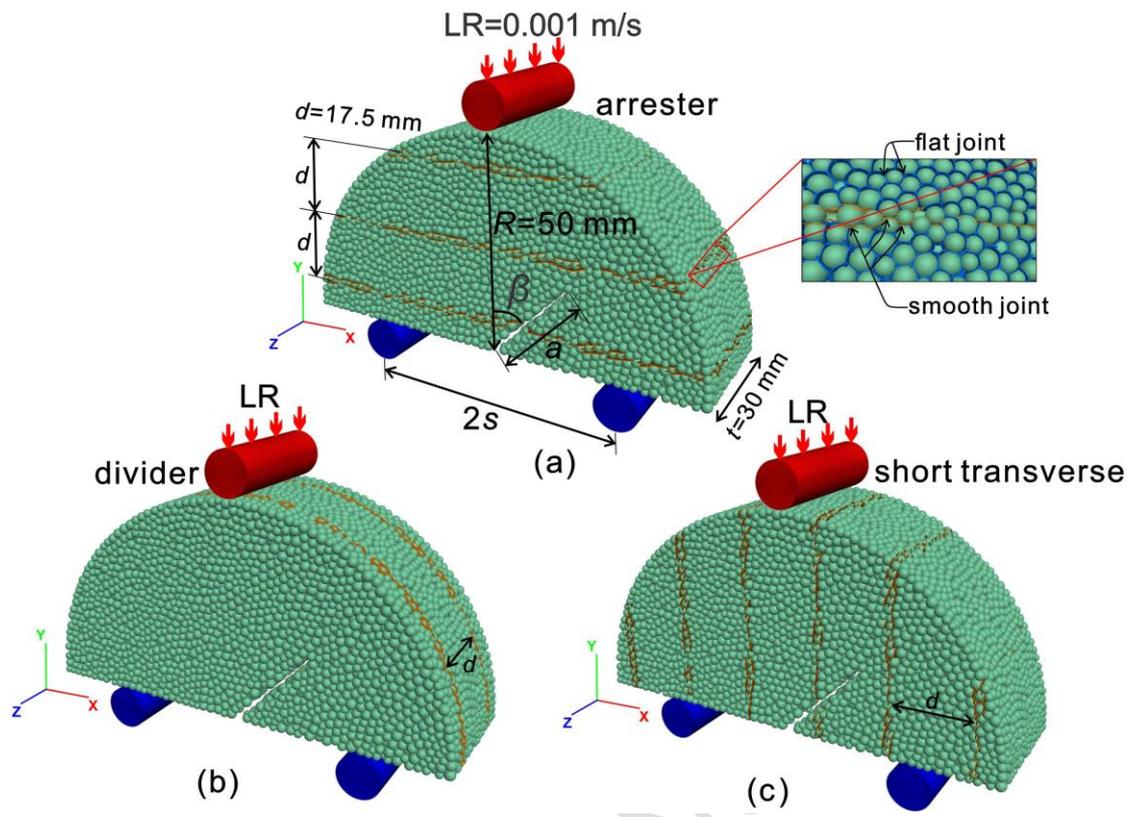
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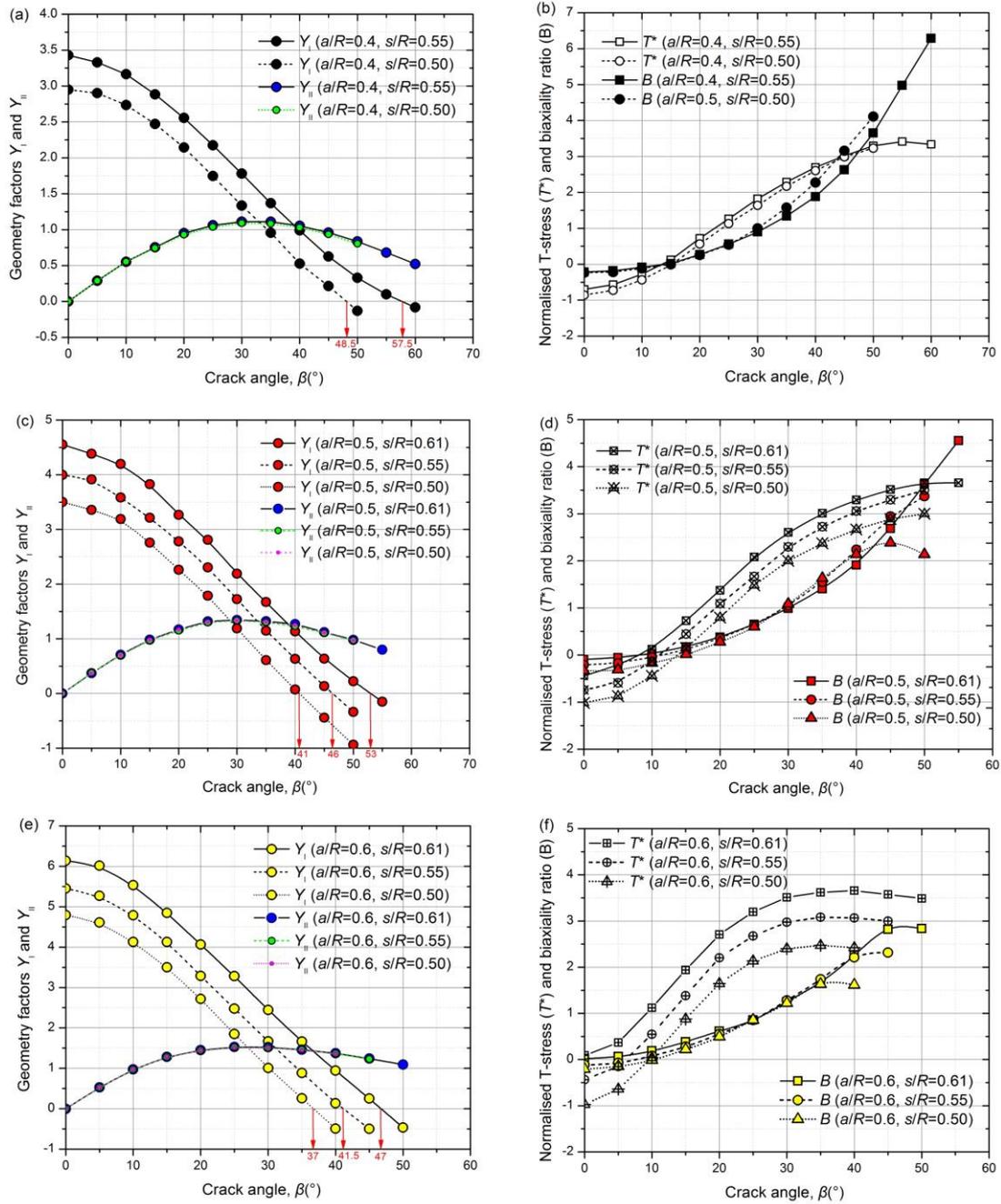


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**Fig 2**

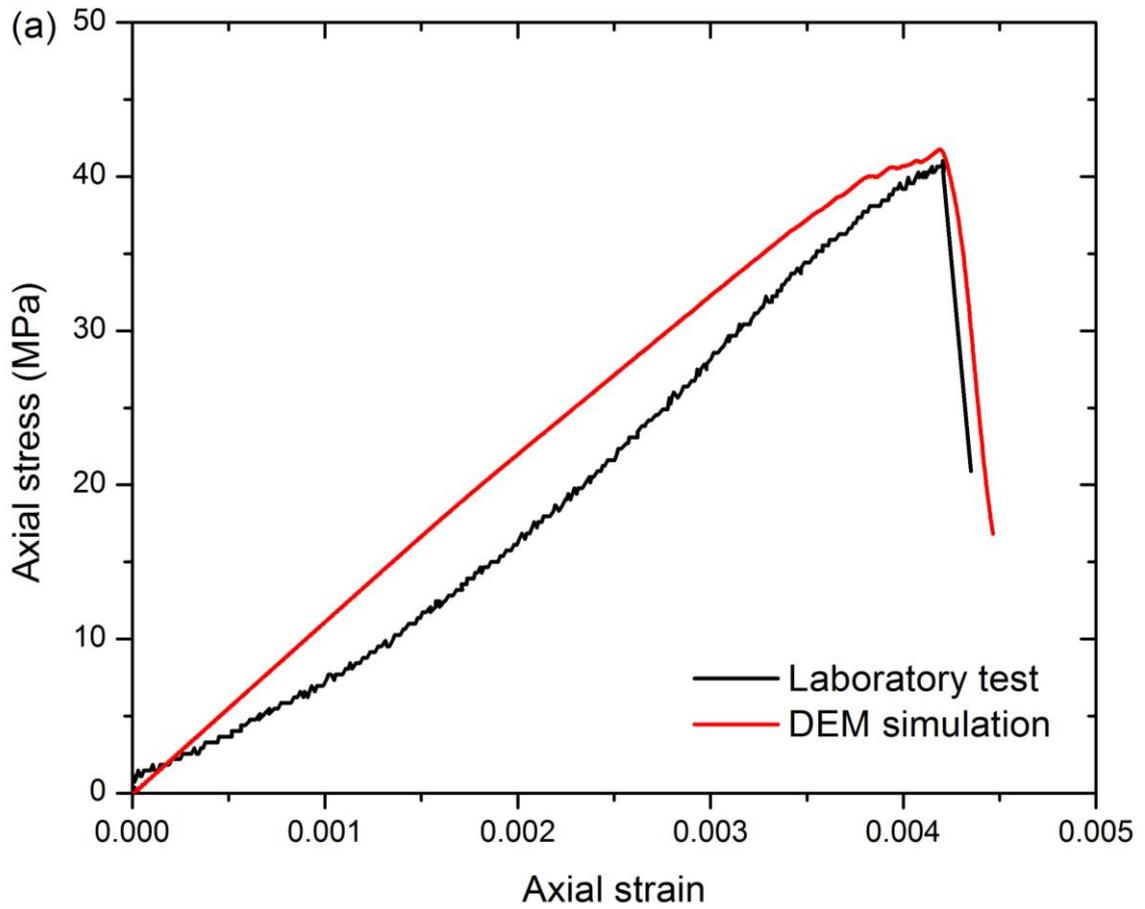
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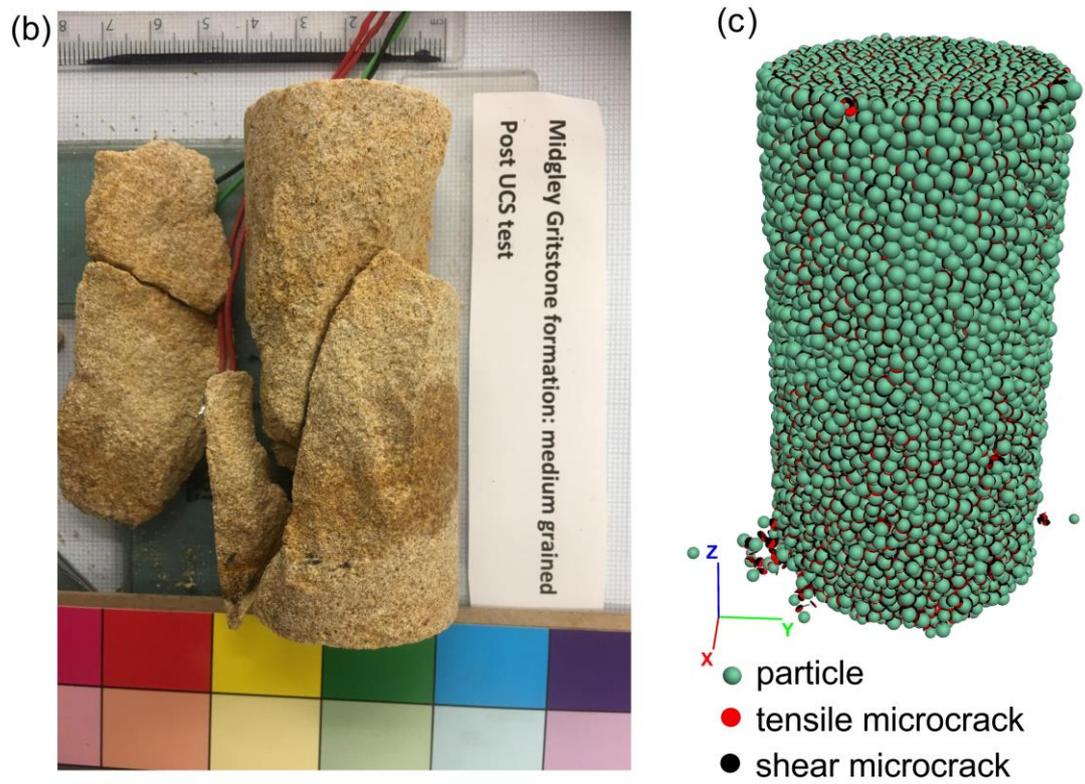
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Fig 3



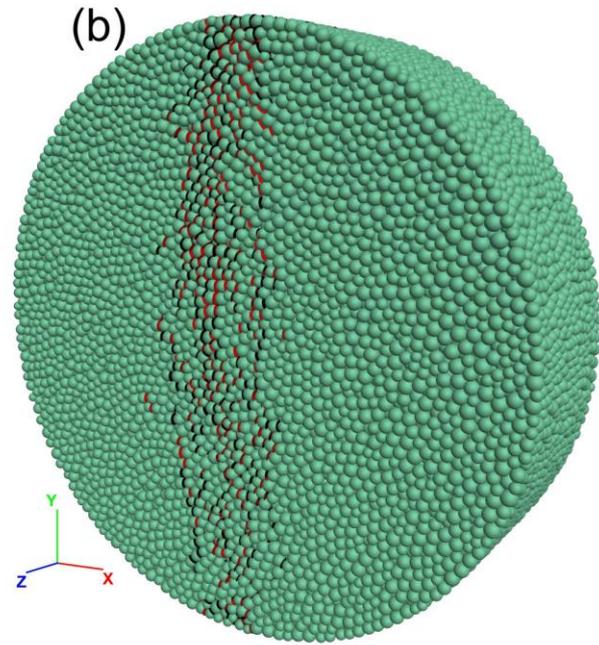
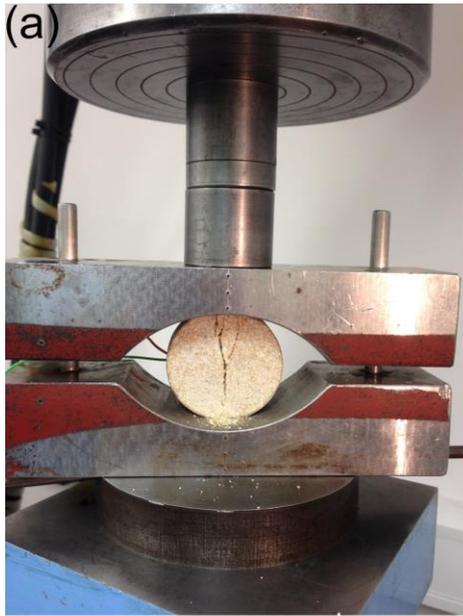
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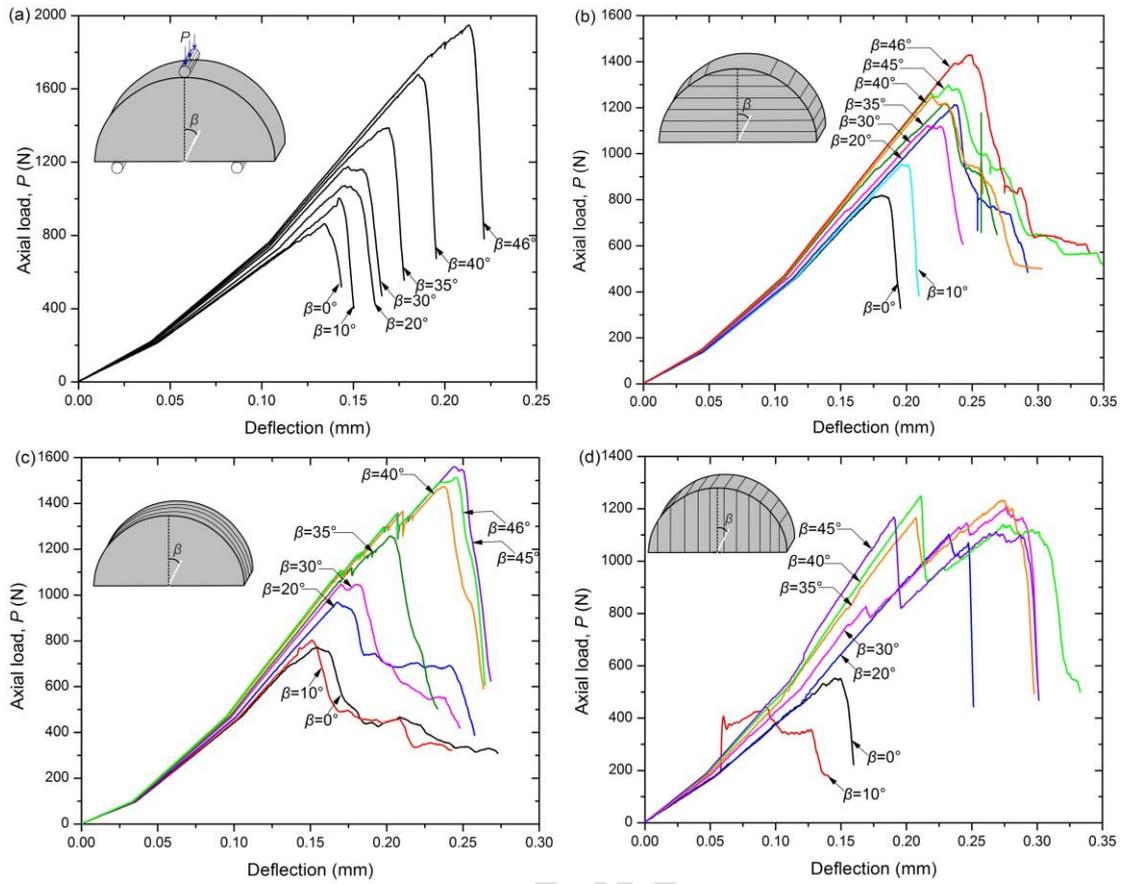
937 **Fig 5**

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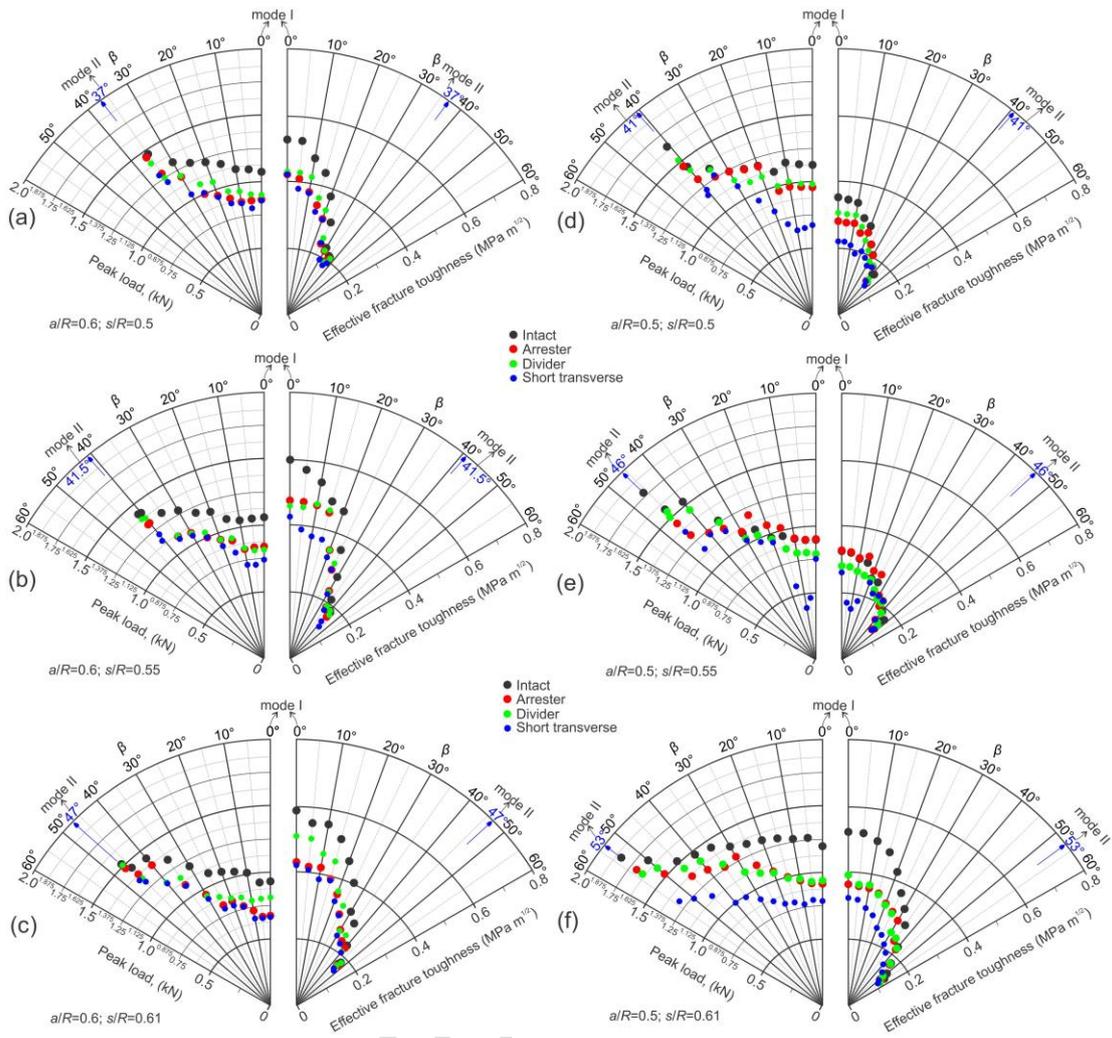
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942 **Fig 6**

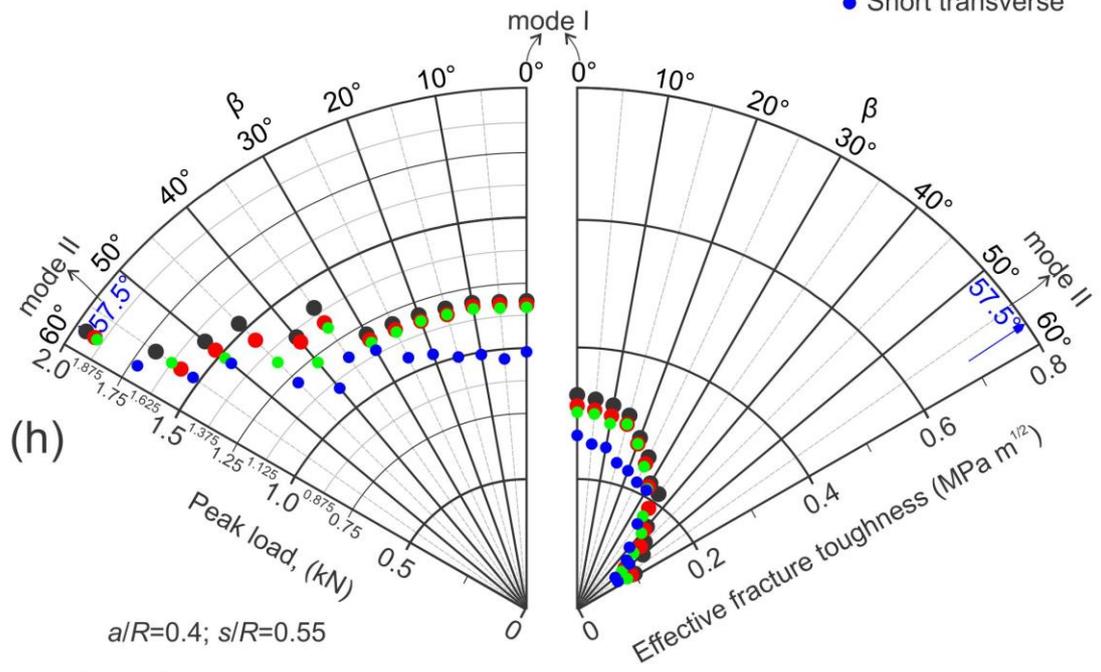
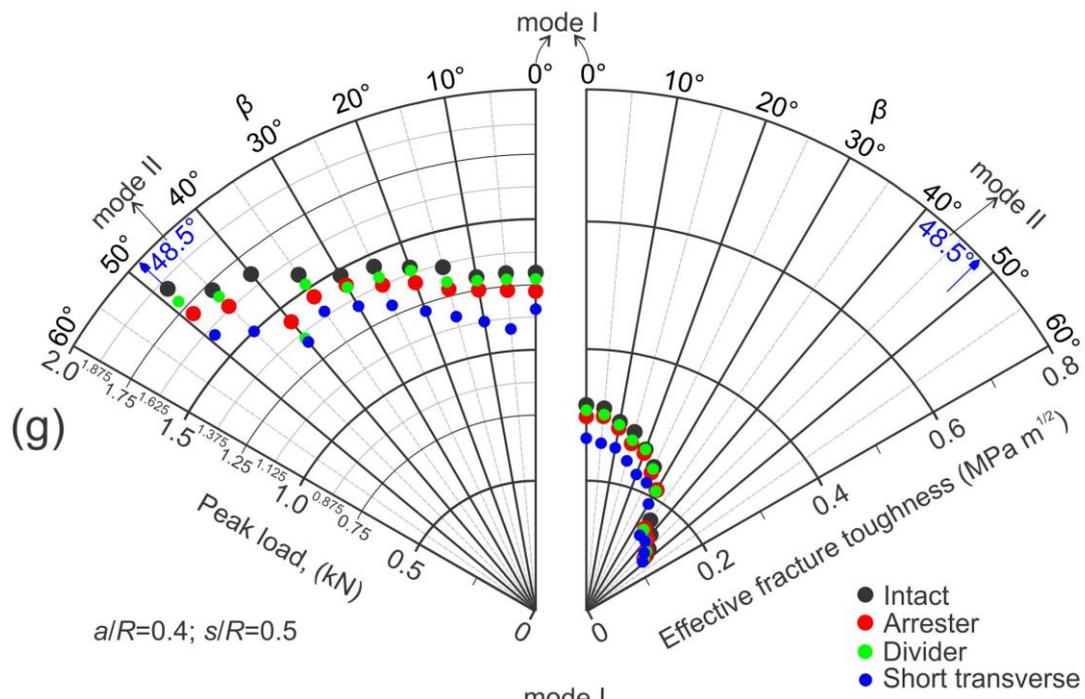
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944 **Fig 7**

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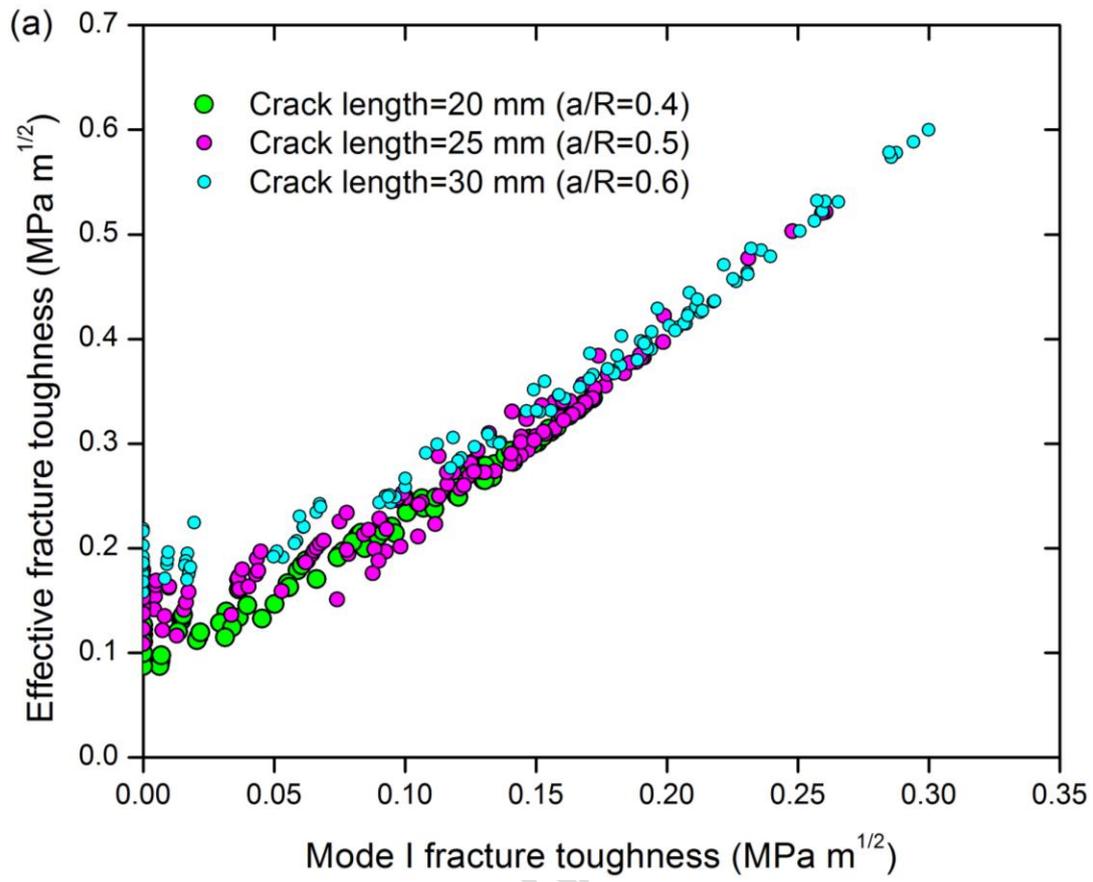
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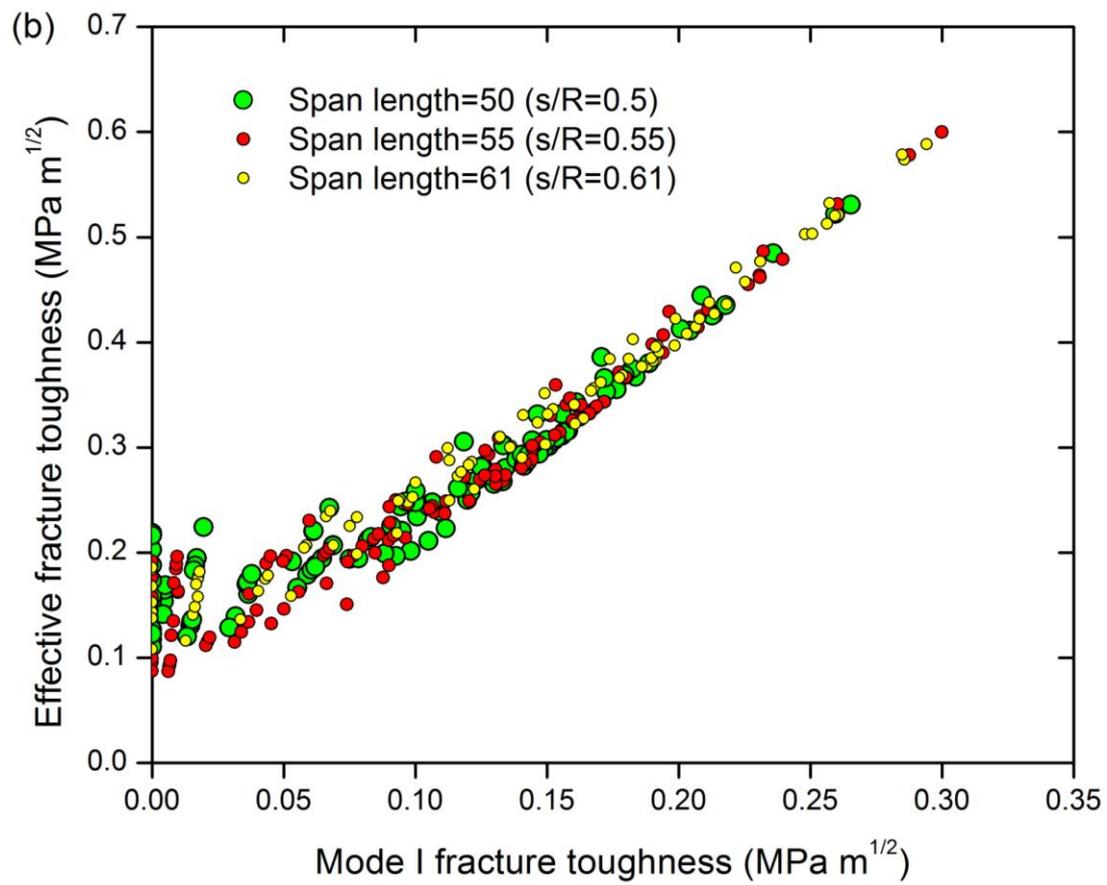


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954 **Fig 8a**

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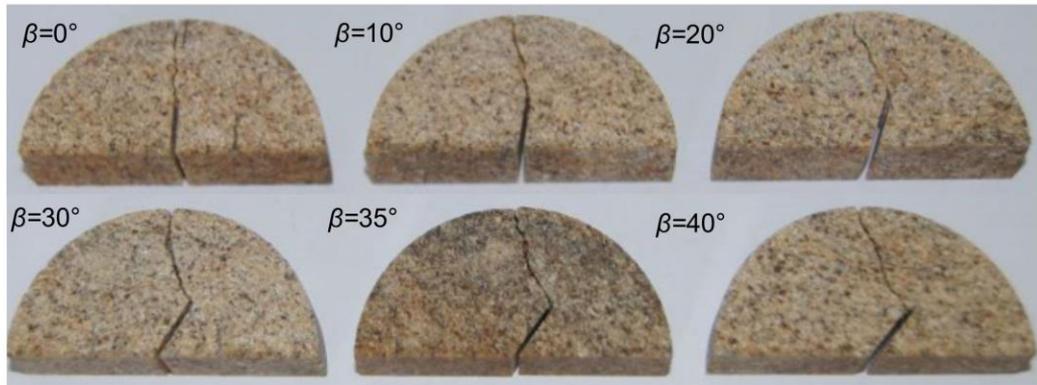
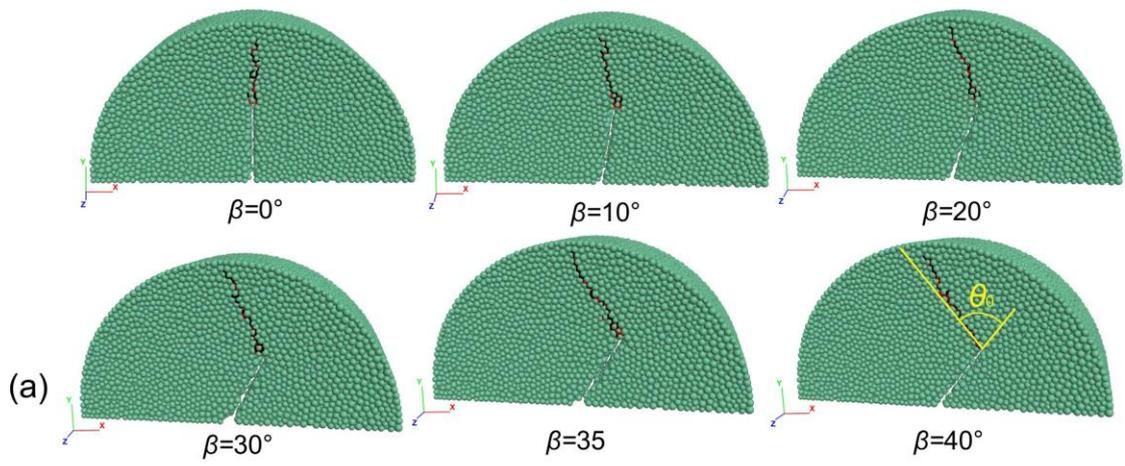
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958 **Fig 8b**

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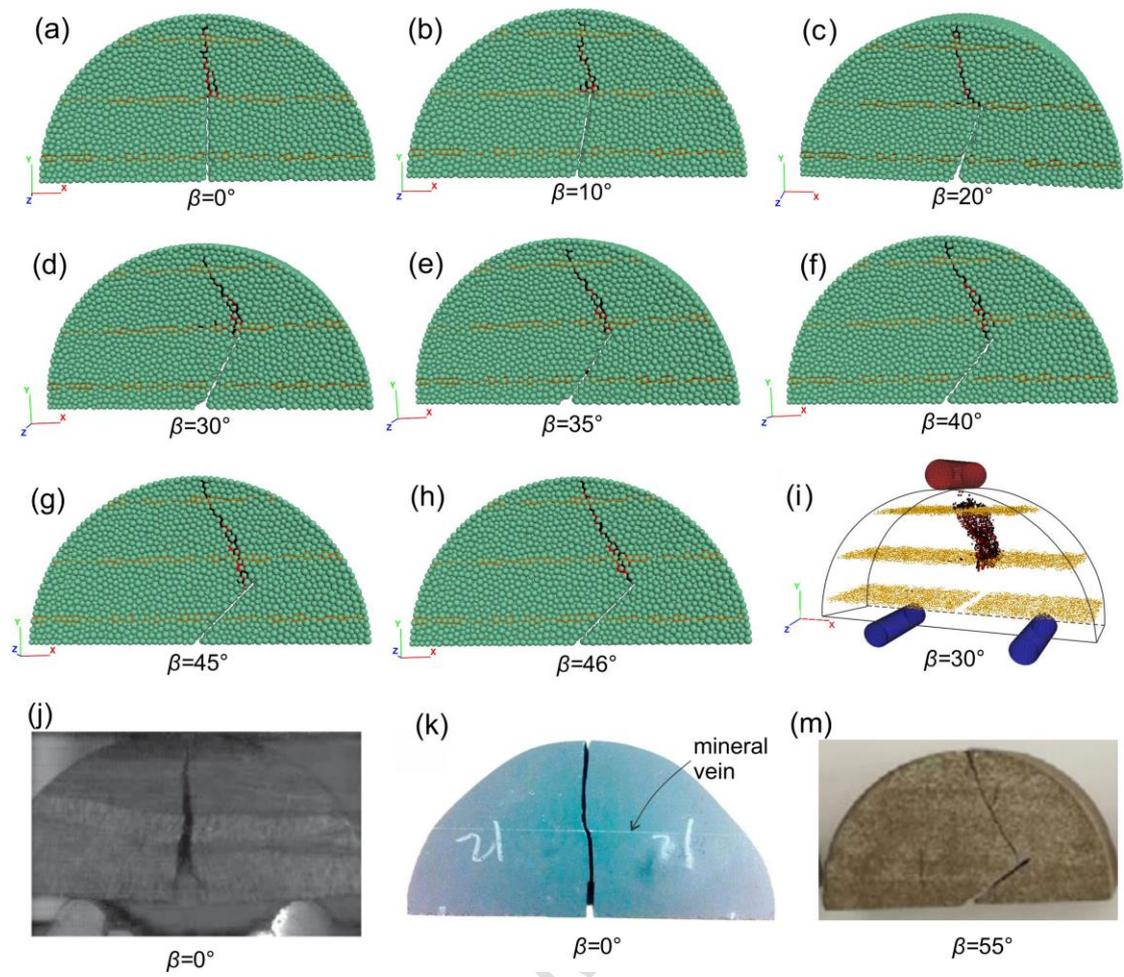


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**Fig 9**

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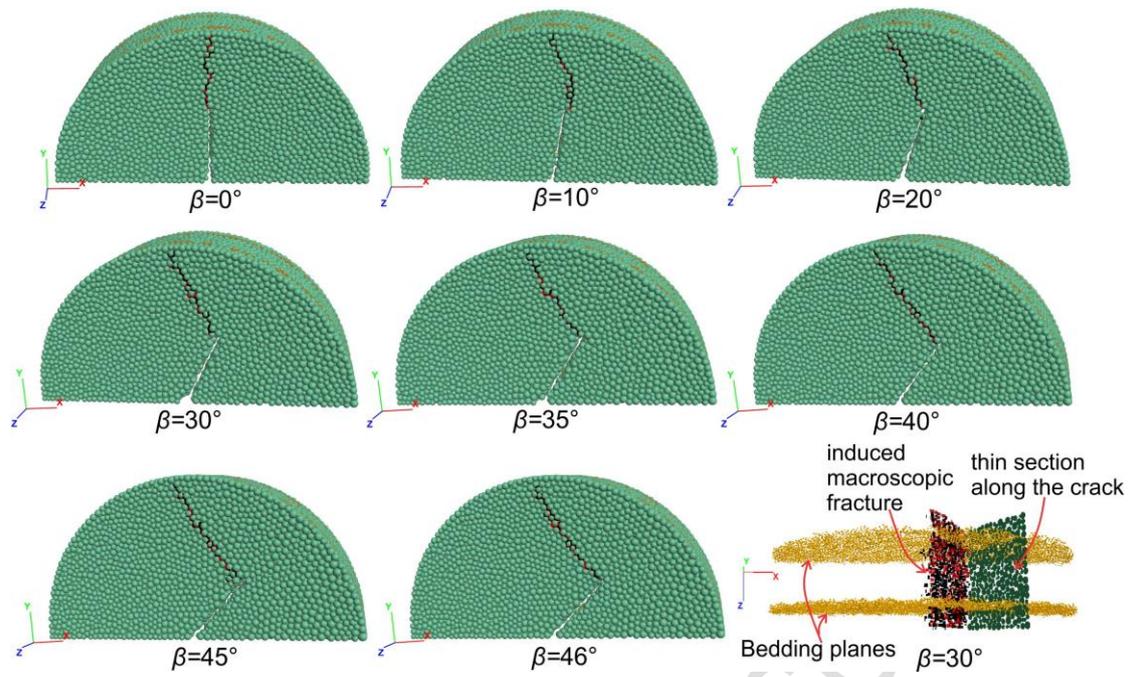


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962 **Fig 10**

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970 **Fig 11**

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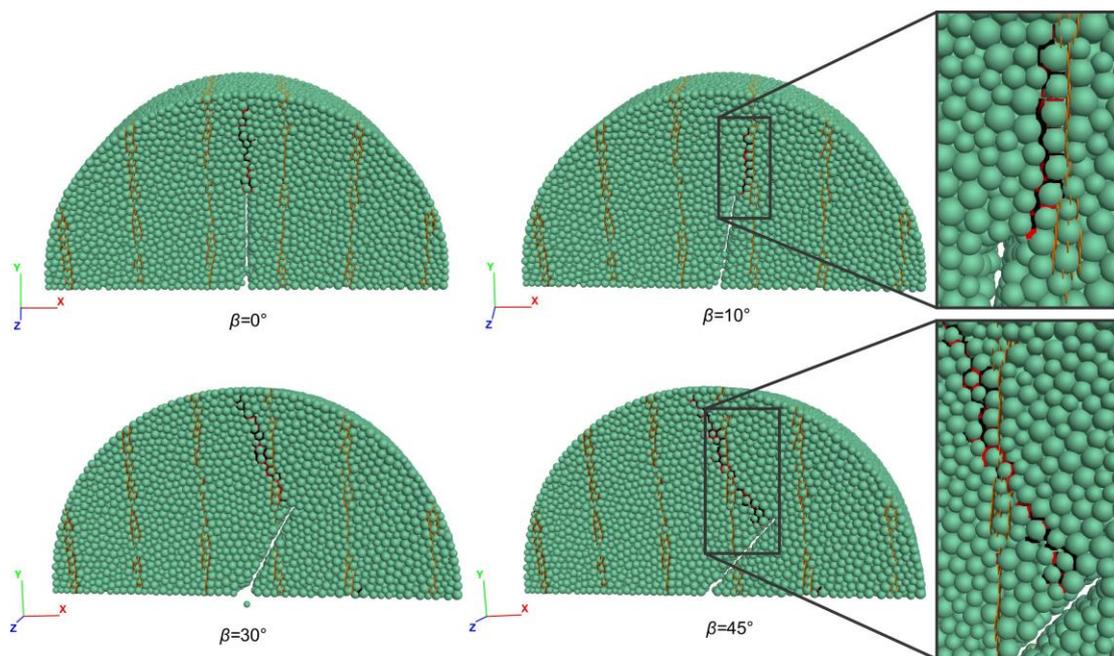
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978 **Fig 12**

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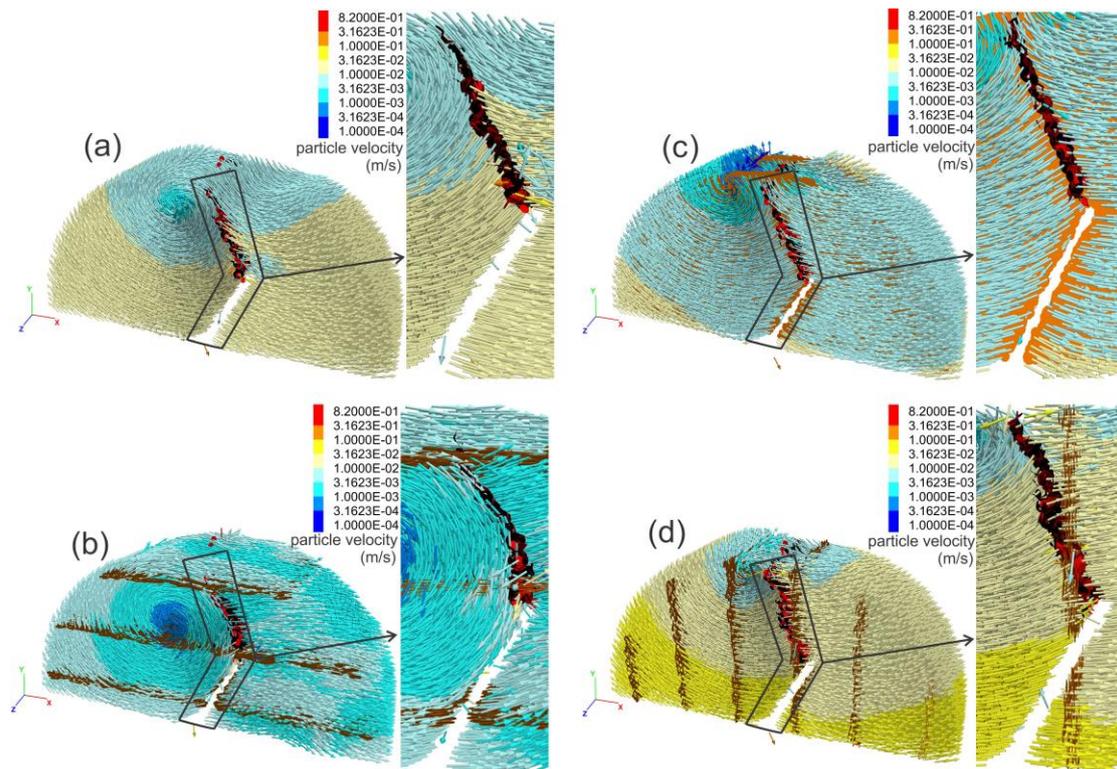
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985 **Fig 13**

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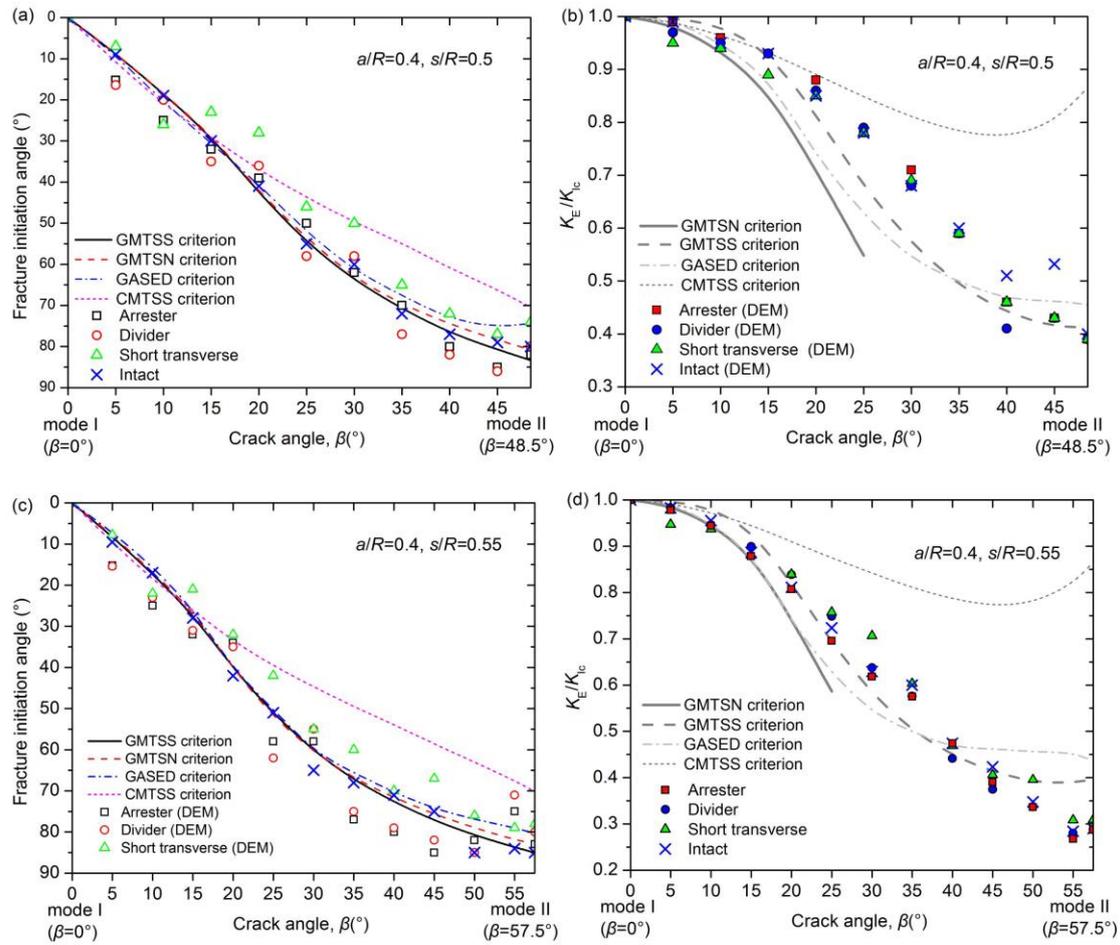
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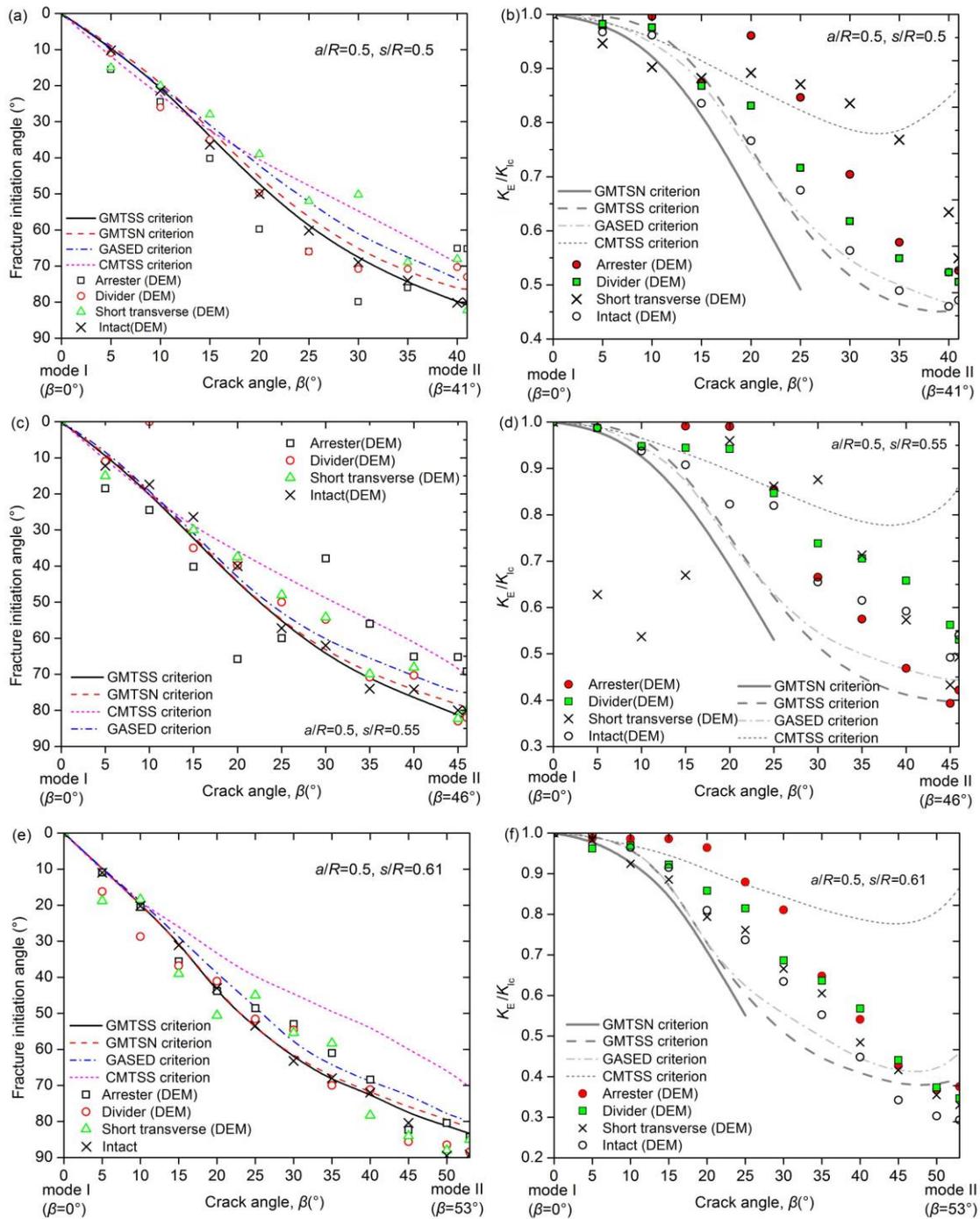
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996 **Fig 14**

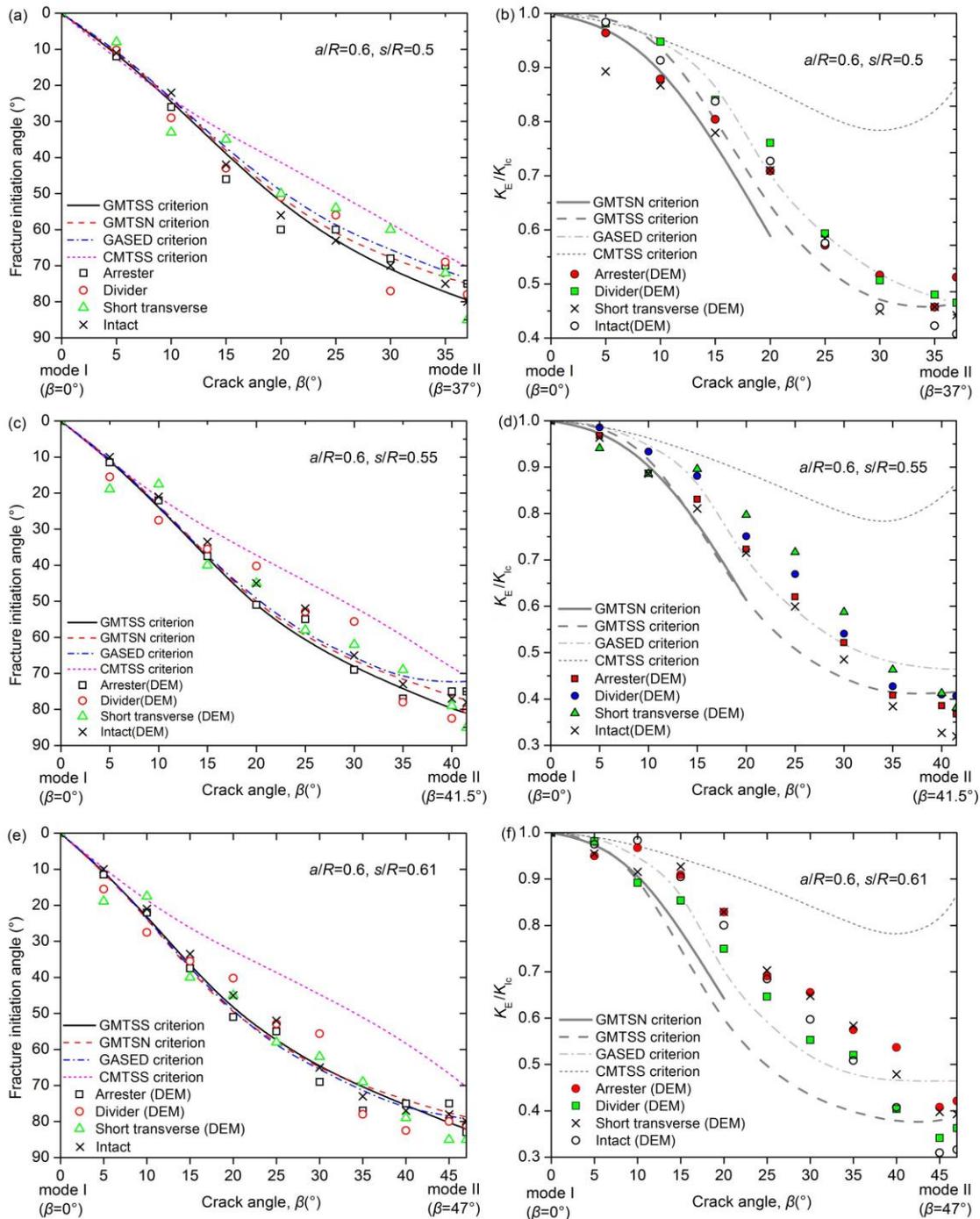
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998 **Fig 15**

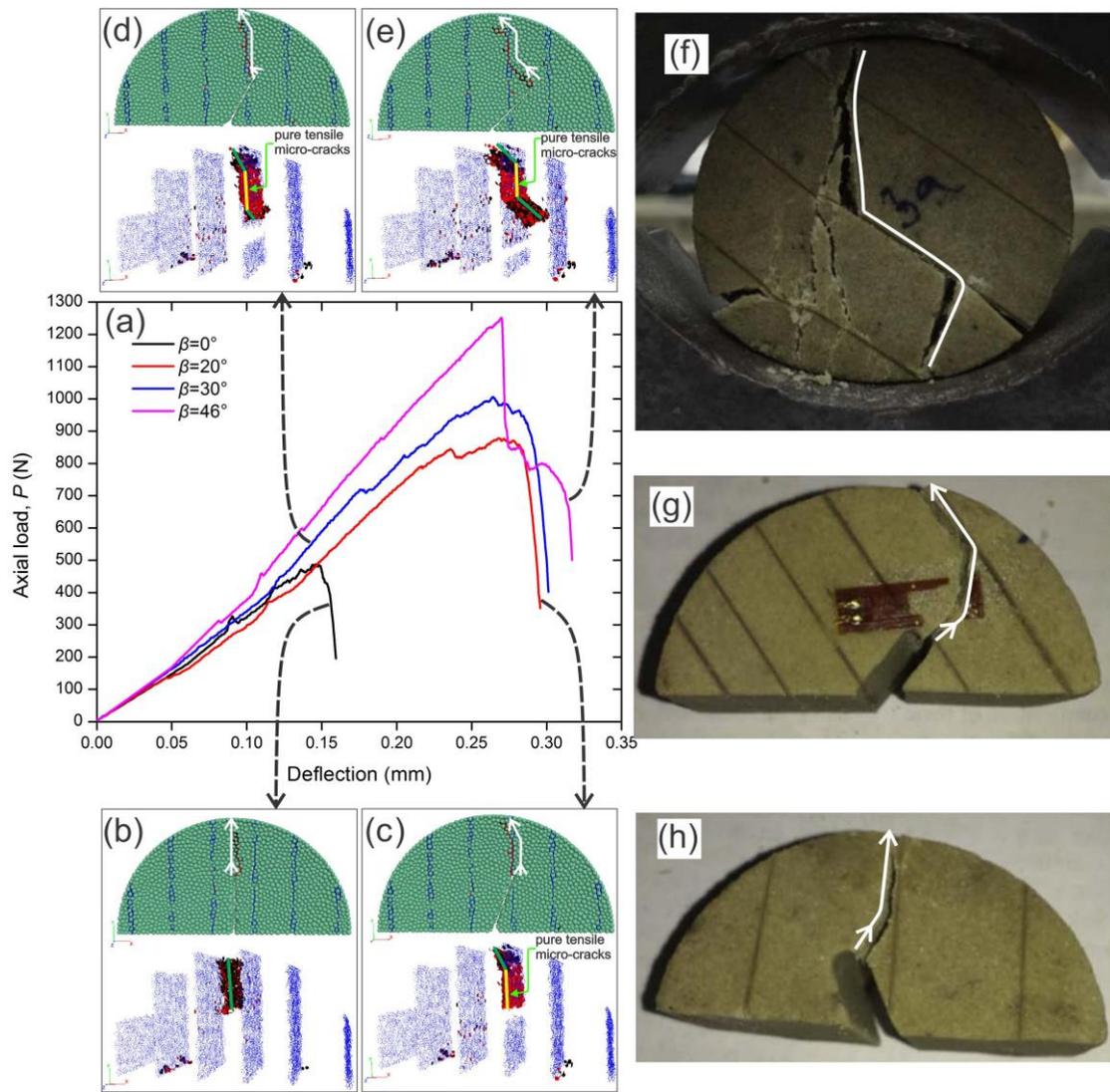
999



1000

1001 **Fig 16**

1002



1003

1004 **Fig 17**

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