

Effect of grain scale geometric heterogeneity on tensile stress generation in rock loaded in compression

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ABSTRACT: Brittle failure of rock is dominated by tensile mechanisms even in an overall compressive stress field. Heterogeneities play a key role in the development of the localized tensile conditions. However, details on how heterogeneities affect brittle rock failure processes are still open for debate. Through the use of regular honeycomb grain arrangements progressing to highly irregular Voronoi arrangements, the impact of grain geometric heterogeneity through finite element tools and discrete element methods was assessed and it is shown that non-uniformity of grain size distribution is not a critical parameter to evaluate crack initiation, peak strength, or micromechanical behaviour. The results demonstrate that grain boundary orientation and grain system arrangements control tensile stress generation inside a brittle rock specimen under compression and thus impact the crack-initiation stress level. This suggests that crack interaction and peak strength is then affected by the kinematic and allowable degrees of freedom in the grain assembly of the damaged rock. At this stage, grain deformability and more importantly grain breakage is needed to increase the degrees of freedom required for the linkage and formation of a macroscopic rupture. Based on this it is suggested that if it is possible to characterize grain boundary orientations or arrangements, various micro-mechanical behaviour could potentially be forecast.

1. INTRODUCTION

Lan *et al.* [1] have reported results for an investigation into the effect of grain heterogeneity on brittle rock failure. They suggest: (1) homogeneous grain size distributions result in higher strengths and that the peak strength is highly dependent on the heterogeneity induced by grain geometry and not by material properties (i.e. modulus contrasts between mineral grains); (2) the minor principal stress is more uniformly distributed in the homogeneous model leading to higher strengths; (3) the geometric variation in grain size and shape induces a large tensile stress-field at relatively low strains when a rock is subject to compressive stresses; (4) geometric heterogeneity has a dominant effect on crack initiation, growth and interaction; and (5) grain size distribution in materials such as brittle rock may be a good index for representing the micro-heterogeneity.

A careful review of Lan *et al.*'s analyses suggest that their conclusions are bias because they used a regular Voronoi tessellation (i.e. honeycomb geometry) as their homogeneous model grain geometry and a single loading direction. The honeycomb geometry is anisotropic and the direction of loading highly impacts

model behaviour. The single loading direction evaluated in [1] is such that little tensile stress is generated along grain boundaries. This is significant because the grains were not breakable and the failure behavior is highly dependent on the ability of grain boundaries to break. In the author's view, this led to biased conclusions suggesting that homogeneous geometries or uniform grain size distributions lead to low magnitude tensile stress conditions and high crack initiation stress levels.

The results presented here provide evidence in support of some findings from [1] and improve the understanding of grain geometry heterogeneity on tensile stress generation.

First, the influence of the anisotropic Voronoi geometry is assessed using finite element methods. Then, a calibrated particle based discrete element method is used to simulate and compare heterogeneous and homogeneous grain structures with breakable and non-breakable grains.

2. REGULAR VORONOI GEOMETRY

The two extreme anisotropic loading directions for a regular Voronoi honeycomb geometry are illustrated in Figure 1; where the (1a) geometry has a high potential to generate tensile conditions along grain boundaries parallel to the direction of loading; and (1b) has a low potential to generate tensile conditions along grain boundaries. The arrangement illustrated in Figure 1b was used by [1] to investigate the influence of grain size heterogeneity.

[1] primarily assessed the influence of grain size heterogeneity using minor principal stress magnitudes and distribution. Here, the magnitude and distribution of the minor principal stress is assessed for the two regular Voronoi geometries using the finite element method implemented in the program Phase² [2]. The samples modeled were 10 cm x 5 cm (h x w) with average grain size of 3.5 mm. The lower boundary was restrained in the y-direction and the model was deformed using displacement boundaries under uniaxial compression. A displacement of 0.1 mm per stage was applied (stages are used for reference). The material properties are summarized in Table 1. The models were elastic and the grains all have the same elastic properties.

The development of tensile stress through the centre of the two regular arrangements with increasing applied displacement (Figures 2 and 3) suggests that only negative (tensile) minor principal stresses develop along the plane of symmetry for the Voronoi cell in Figure 2 (tensile geometry). For the Voronoi cell in Figure 3 (non-tensile geometry) both positive and negative minor principal stress magnitudes develop with positive minor principal stress developed along grain boundaries. The rate of tensile stress development is greater for the tensile geometry (Figure 2) where at stage 8 (0.7 mm of applied axial deformation) the tensile stress magnitude nears -6 MPa and ranges from approximately -2 MPa to -6 MPa whereas the tensile stress in the non-tensile geometry (Figure 3) is significantly lower and not as rapidly developing; > -2 MPa ranging approximately between +2 MPa to > -2 MPa. The minor principal stress distribution in Figure 3 is similar to the results from [1] for the same geometry (Figure 12 in [1]) suggesting that these models can be used for comparative purposes.

The results presented here clearly demonstrate that the two anisotropic Voronoi arrangements develop a uniform distribution of stress as found by [1] but the results also show that the arrangement assessed by [1] is in fact biased towards low tensile stress generation along grain boundaries.

Most importantly, the arrangement has low tensile stress generation potential at low strains. This is significant

because only grain boundary breakage was allowed in [1].

Next, the development of tensile stress relative to deformation of a sample subject to uniaxial compression for regular and irregular Voronoi tessellations is investigated.

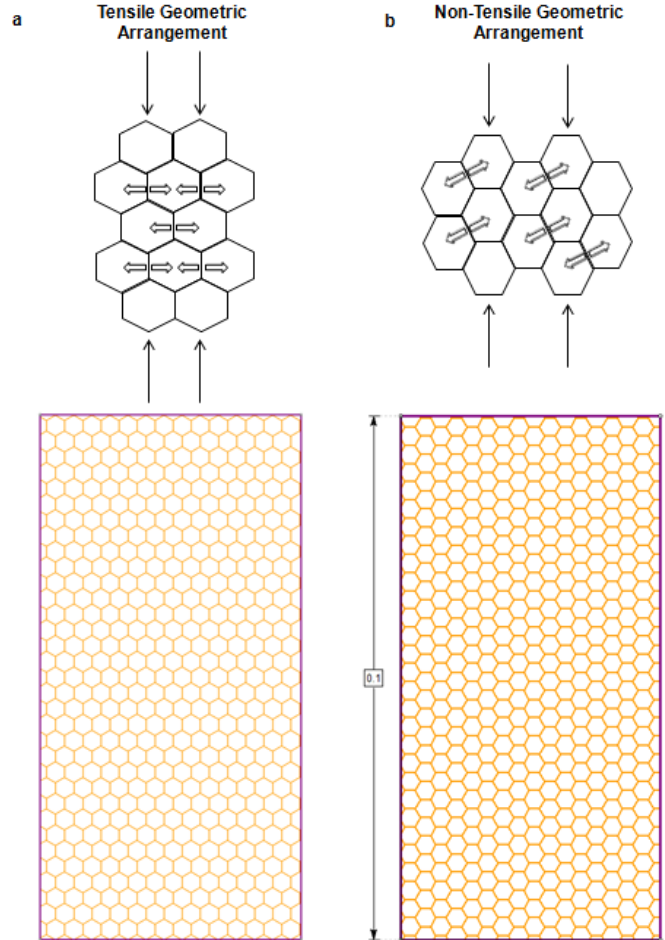


Fig. 1. Geometric arrangements for the end member anisotropic orientations for regular honeycomb Voronoi tessellations.

Table 1: Finite element simulation material properties

Mesh Properties	
Young's Modulus, E (MPa)	90,000
Poisson's Ratio, ν	0.25
Joint Element Properties	
Normal Stiffness (MPa/m)	700,000
Shear Stiffness (MPa/m)	70,000

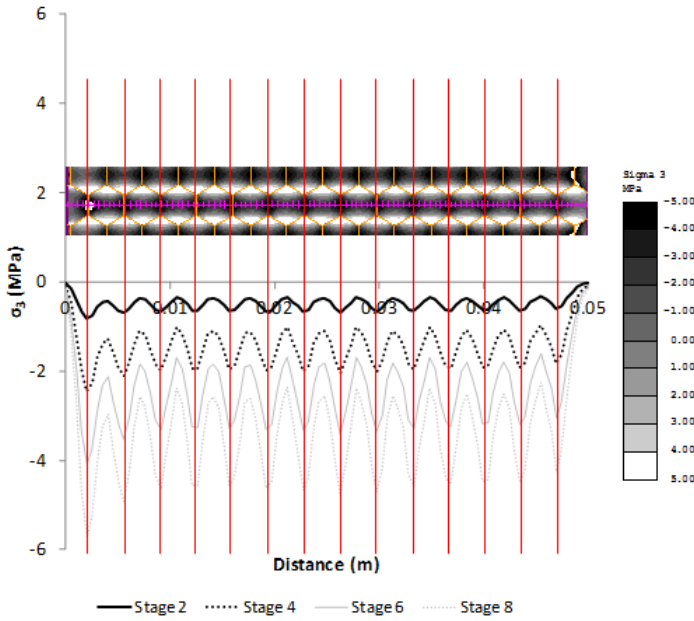


Fig. 2. Development of tensile stress in the preferential tensile geometric arrangement with increasing applied displacement.

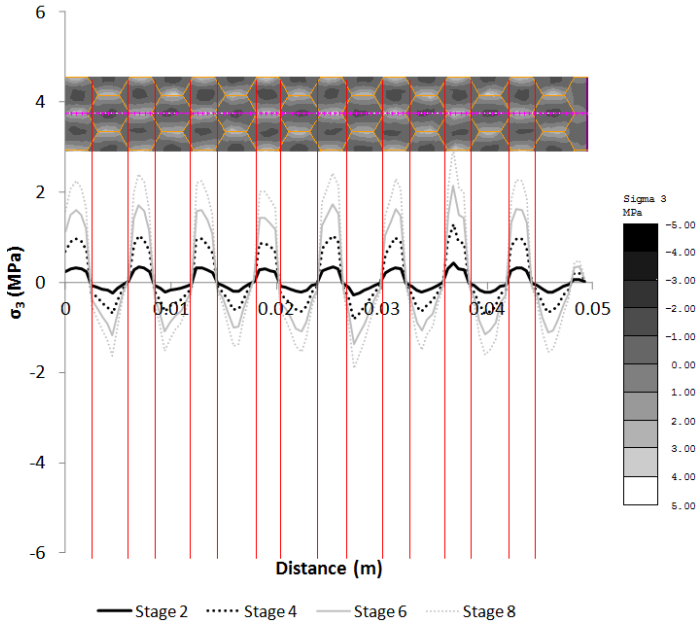


Fig. 3. Development of tensile stress in the non-preferential tensile geometric arrangement with increasing applied displacement.

3. TENSILE STRESS DEVELOPMENT, GRAIN HETEROGENEITY AND STRAIN-SENSITIVITY

The two anisotropic Voronoi tessellations are used to assess the influence of increasing tessellation irregularity on the development of tensile stress with increasing axial strain. The same model size, boundary conditions and elastic material properties were used as previously described. The grain geometric arrangements progressed from Set 1: the regular tensile geometric arrangement to irregular arrangement, Figure 5, referred to as 1a to 1d;

and Set 2: regular non-tensile geometric arrangement to irregular arrangement, Figure 6, referred to as 2a to 2d.

The grain size distributions for each of the model sets are shown in Figure 4. The regular (1a and 2a), slightly irregular (1b and 2b) and moderately irregular (1c and 2c) sets all have relatively uniform grain size distributions. The highly irregular Voronoi tessellations (1d and 2d) have more graded distributions (more heterogeneous grain size).

The magnitude of tensile stress development versus stage was monitored at select points along grain boundaries for each model. The selected points were high tensile stress generating zones which are indicated in Figures 5 and 6 (red ovals). The results of the assessment (Figure 7) suggest that all models have a similar magnitude of tensile stress generation at the selected points except for the regular Voronoi tessellation that produces the least tensile stress (2a, same grain geometry assessed by [1]). This is consistent with previous conclusions. Model 2a (non-tensile geometry) responds to deformation in a distinctly different manner when compared to all other models. While only one point was monitored in the models, assessment of the overall average minor principal stress in the samples resulted in the same conclusion.

All of the regions monitored to generate the results presented in Figure 7 have arrangements similar to the ideal linear elastic model presented by [3] except for Set 2 Regular (model 2a) which is not in a geometric arrangement to generate significant grain boundary tensile stress conditions. This observation is also supported by [1] (Figure 13 in [1]) where, while not mentioned in the journal article, the contacts associated with their 'Model 2' (irregular) are preferentially associated with linear elastic model geometries.

Grain boundary stiffness values were also increased to $k_n=2,000,000$ MPa/m and $k_s=200,000$ MPa/m. Stiffer boundaries resulted in faster rates of tensile stress development.

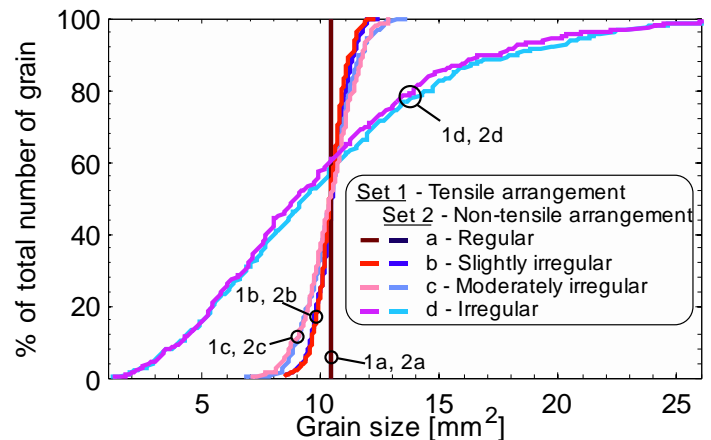


Fig. 4 Grain size distributions for each model Set.

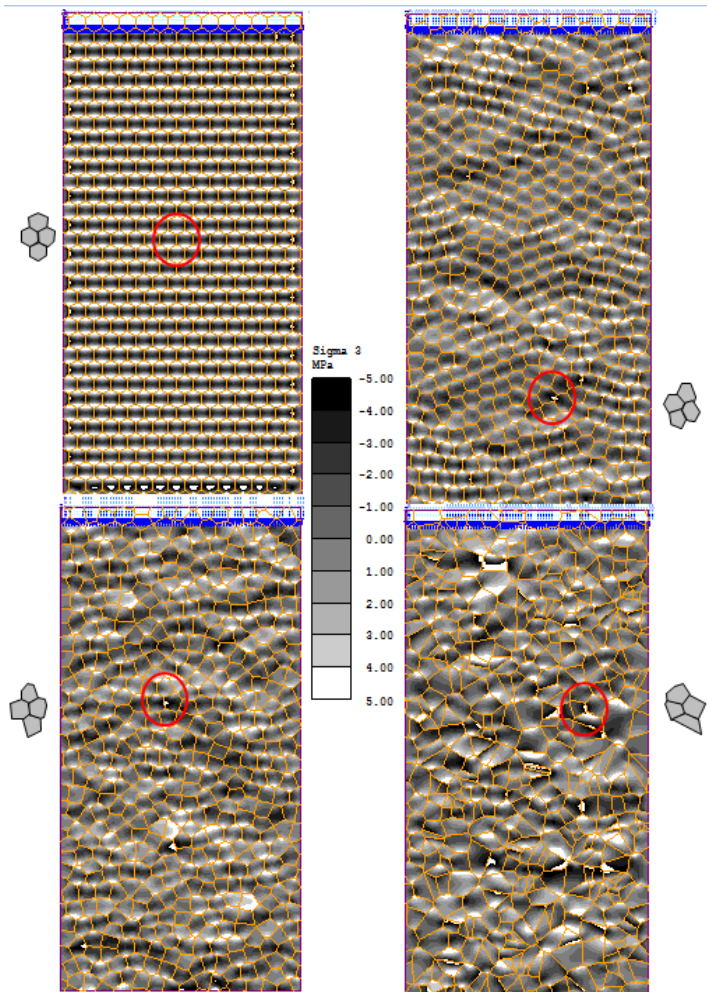


Fig. 5. Set 1 regular to irregular Voronoi tessellation. Red inset shows selected grain arrangements generating tensile conditions (grey schematics). Used for tensile stress magnitude plots in Figure 7. Contouring of minor principal stress (black to white contour is more tensile).

4. TENSILE STRESS AND GRAIN BOUNDARY ORIENTATION

The distribution of grain boundary orientation for each model is given in Figure 8a. The two regular models (1a and 2a) have distinct grain boundary orientations. All other models have similar grain boundary orientation distributions with no obvious preferential orientation of the boundaries.

The distribution of minor principal stress along grain boundaries for stage 8 (0.7 mm of applied displacement) is shown on Figure 8b. All irregular models have similar stress distributions. The regular models have step like distributions. Model 1a (tensile arrangement) spans a stress range similar to the irregular models while model 2a spans a narrower range and is less tensile.

When comparing Figures 4, 8a and 8b, it is evident that the parameter controlling the stress distribution at the grain boundary is the grain boundary orientation and not the grain size distribution.

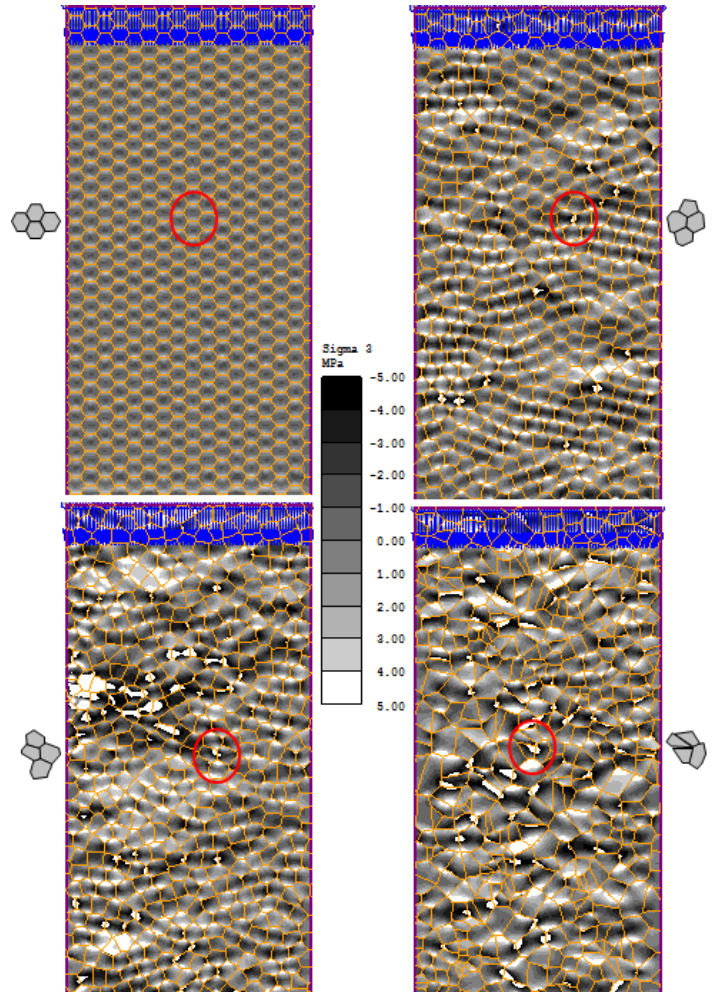


Fig. 6. Set 2 progressing from regular to irregular Voronoi tessellation. Red insets show selected grain arrangements generating tensile conditions (grey schematics). Used for tensile stress magnitude plot in Figure 7. Contouring of minor principal stress (black to white contour is more tensile).

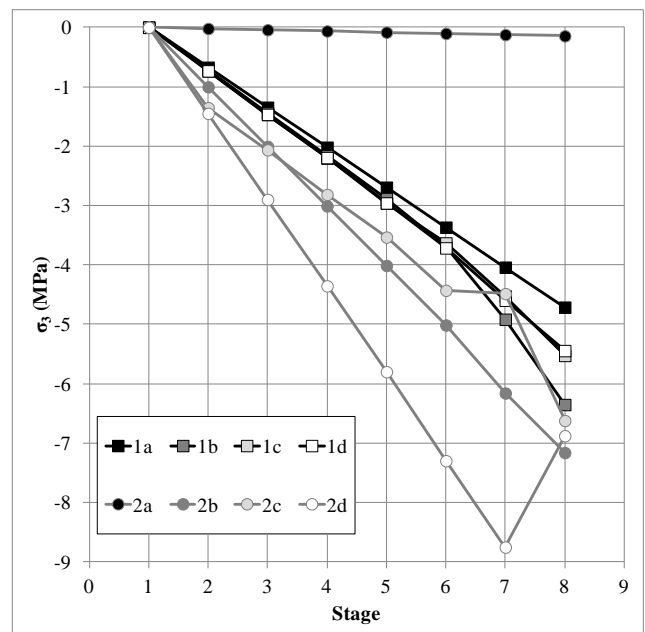


Fig. 7. Tensile stress development along grain boundaries in Set 1 and Set 2 models. Deviation from straight lines due to grain boundary kinematics.

If grain size distribution was more important, Models 1d and 2d would have distinct stress distributions compared to the other models since they have distinct grain size distributions. The single model that shows a distinct stress distribution is model 2a. What makes model 2a distinct from all other models is that it is the only model that has no grain boundaries oriented parallel to the loading direction.

Figure 9 plots the minor principal stress along grain boundaries as a function of grain boundary orientation for model 2b, which is representative of all other models except model 2a (regular non-tensile case). Early in the loading history, Figure 9a, tensile stresses build on grain boundaries which are within $\pm 20^\circ$ of the loading direction. With increasing deformation, Figure 9b, the distribution of stress versus grain boundary angle becomes asymmetric. Generally, three domains can be identified based on grain orientation: (1) grain boundaries within $\pm 25^\circ$ of the loading direction are tensile (large magnitude); (2) grain boundaries at angles from 25° to 90° of the loading direction are in slight compression; and (3) grain boundaries between 90° and 155° of the loading direction are in slight tension.

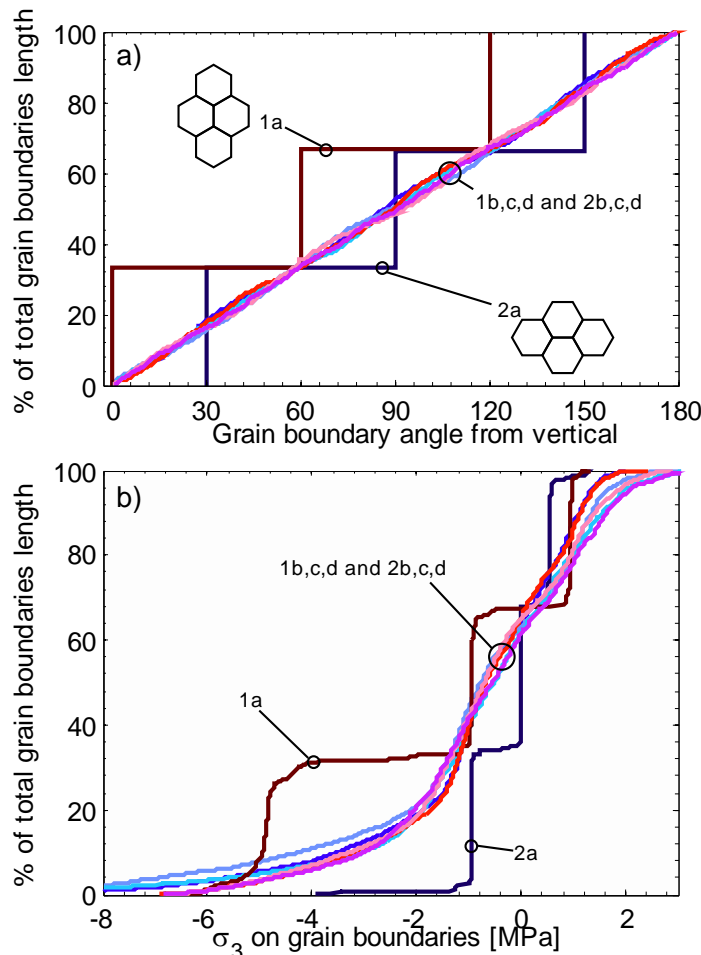


Fig. 8. Grain boundary orientation distributions for Set 1 and 2 models (a). Minor principal stress magnitude along grain boundaries for Set 1 and 2 models at stage 8(b).

This distribution can be explained by considering the kinematics of the deformation as presented in the insert of Figure 9b. Shear develops on critically oriented boundaries. A preferential shear direction that can be dextral or sinistral develops, probably controlled by slight variation in initial grain structure geometry. This shearing induces further extension on the boundary sub-parallel to the loading direction as well as secondary extension on the conjugate planes.

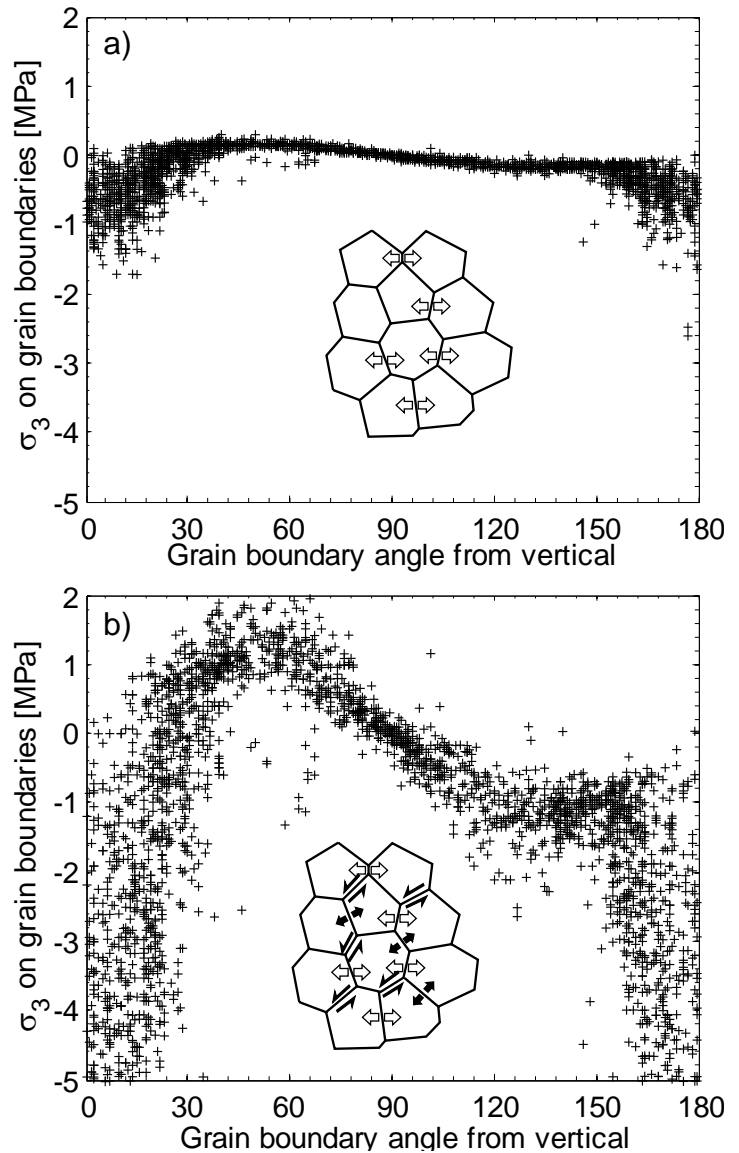


Fig.9. Minor principal stress along grain boundaries, model 2b, stage 2 (a) and stage 8 (b).

5. BREAKABLE VERSUS NON-BREAKABLE GRAIN STRUCTURES

Next, a single set of results generated using the Particle Flow Code, PFC^{2D} [4] and the developed Grain-based Model (GBM) [5] is presented to illustrate the impact of grain breakage. While only a limited number of conclusions can be drawn from a small number of simulations, the results do clearly show that grain size heterogeneity is not as critical as grain boundary orientation heterogeneity.

A set of models with heterogeneous breakable grains was calibrated to low confinement failure process conditions (uniaxial compression, direct tension and direct shear up to 40 MPa normal stress). This model was used to simulate both heterogeneous and homogeneous grain structures with breakable and non-breakable grains. The rock simulated is a low porosity (<2%) hard brittle sandstone (consisting of 50% feldspar, 20% quartz, and 30% calcite cementation) which behaves as a typical brittle rock. This heterogeneous calibrated model was then modified such that its grain structure was homogeneous and/or with non-breakable grains to investigate these effects on peak strength (uniaxial compression and direct tension), and modulus. The results are also compared with respect to crack initiation (CI) as determined using the methodology from [6]. Since, the models were not calibrated to CI and CI from [6] is only a qualitative parameter, the CI results are only used for a relative comparison. The grain size distributions and simulated grains structures are shown in Figure 10.

The model results are summarized in Table 2 and show that when breakable grains are considered, heterogeneous or homogeneous grain size distributions do not significantly influence the results with respect to peak strength, modulus, crack initiation or direct tensile strength. For unbreakable grains, the peak strength is significantly increased, 29% (consistent with the findings of [1]) but the modulus, crack initiation stress level and direct tensile strength are only slightly influenced. This finding is in contrast to [1] and is likely due to the non-regular homogeneous modified-Voronoi tessellation used in the PFC^{2D} simulation oppose to the regular low tensile generating geometry used by [1].

Table 2: Influence of heterogeneity and breakability

Model	Grain Structure	Failure Allowed	UCS (MPa)	Young's Modulus (MPa)	CI* (%UCS)	Direct Tensile Strength (MPa)
1	Hetero.	Grain and Boundary	125	46725	42	-16.6
2	Homo.	Grain and Boundary	120	45382	51	-17.5
3	Hetero.	Boundary	205	35687	16	-10.4
4	Homo.	Boundary	264	39777	14	-9.5

*Crack Initiation as per [6]

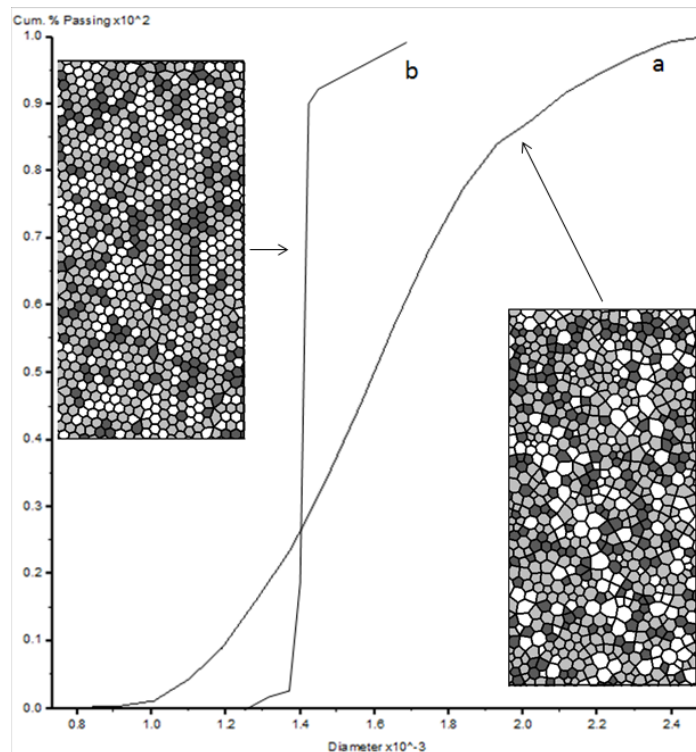


Fig. 10 Grain size distributions heterogeneous (a) and homogeneous (b) for PFC^{2D} GBMs. The structures have the same average grain size (~1.4mm). Simulated grain structures also shown. Dark grey – quartz, light grey – feldspar, white – calcite.

6. DISCUSSION

The geometrical arrangement and relative orientation of grains in a rock (rock fabric) has been used to assess various rock properties such as some ductile characteristics [7], fracture strength [8,9], linear compressibility [10], thermal expansion [10], and thermal conductivity[10].

Grain boundary orientation controls the development of tensile stress (rate and magnitude) at the grain scale. Grain boundary cracking has been proposed to be the dominate mechanism active at crack initiation [11]. If grain boundary orientations could be characterized (or linked to rock fabric), brittle rock characteristic behaviour such as crack initiation could potentially be estimated or used for assessment of rock brittleness.

7. CONCLUSIONS

The investigation of grain size heterogeneity considering elastic modeling and discrete element modeling using breakable and non-breakable grains has led to the following conclusions:

- Homogeneous grain size distributions with non-breakable grains result in higher strengths. Homogeneous grain sizes distributions with breakable grains result in similar strengths to the heterogeneous simulation. Peak strength is not highly dependent on the heterogeneity induced by grain geometry, it is dependent on the grain strength or intra-grain breakage characteristics.
- The minor principal stress is more uniformly distributed in the homogeneous rocks but does not lead to higher strengths except when the regular Voronoi tessellation with little tension generation potential is adopted. This is a very particular case that is not generally applicable.
- Grain boundary orientation heterogeneity induces large tensile stress-fields at relatively low strains when rock is subject to compressive stresses; it is not the geometric variation in grain size and shape that dominates internal tension developments.
- Geometric heterogeneity qualitatively does not appear to have a dominant effect on tensile crack initiation.
- Grain size distribution in materials such as brittle rock is not a viable index to represent the micro-heterogeneity. Grain boundary orientation is potentially an index for representing the micro-heterogeneity.

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