Fracture Process Simulation Based on Measurements of Fracture Toughness of Mineral Grains and Grain Boundaries.

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1. INTRODUCTION

In this paper, fracture process simulation based on the microscopic and macroscopic fracture toughness of granite was generated in order to understand the fracture process mechanism. For the purpose of this study, the following laboratory experiments and numerical simulations were carried out.

1) SCB(Semi-Circular Bending) tests were carried out in order to determine macroscopic fracture toughness of Inada granite. some experiments were performed using SCB specimens with varying specimen dimensions to verify the size effect of fracture toughness.
2) Micro-sized specimens were prepared in min eral grains and grain boundaries. Microscopi c fracture toughness (described as MFT) tes ts were performed in order to measure the microscopic mechanical properties using for numerical simulations. In particular, some M FT specimens inside grains were also prepar ed in varying the dimensions to verify the size effect.
3) Microscopic parameters in the numerical simulation were calibrated based on micro mechanical properties obtained from MFT tests. SCB simulations were generated from the calibrated microparameters and SCB simulations were carried out on them. Fracture toughness obtained from laboratory SCB tests and numerical simulations were compared and discussed.

2. MACROSCOPIC MECHANICAL PROPERTIES OF INADA GRANITE

Inada granite was used in this study. This rock was produced from Iwase to Inada in Ibaraki Prefecture, Japan. Inada granite was mainly composed of four minerals, quartz, plagioclase, K-feldspar and biotite, as shown in Fig.1.

In order to measure the macroscopic Mode I fracture toughness of Inada granite, SCB tests were performed using SCB specimens with different radius ranging from 15.0mm to 80.5mm.

Fig.2 shows the results of the SCB tests and the relation between specimen radius and Mode I fracture toughness. In general, Bažant size effect law is known as the size effect theory (Bažant et al., 1984), so the black curve in this graph represents the estimated value based on Bažant's law. In this study, for comparison with the value of numerical simulation value, the macroscopic fracture toughness was predicted to be 1.20 [MPa$\sqrt{\mathrm{m}}$].

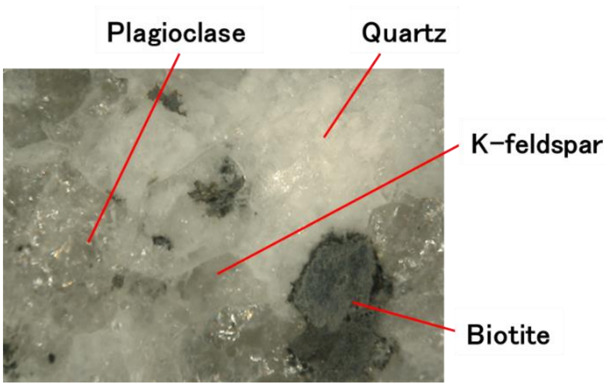


Fig.1 Mineral grains of Inada granite; quartz, plagioclase, K-feldspar, biotite.

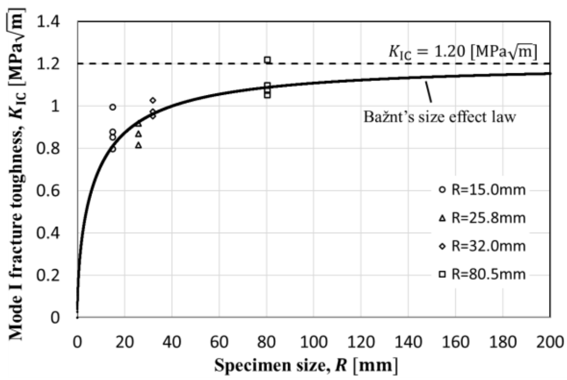


Fig.2 Mode I fracture toughness of Inada granite with various size

3. MICROSCOPIC MECHANICAL PROPERTIES OF MINERAL GRAINS AND GRAIN BOUNDARIES OF INADA GRANITE

In order to obtain the microscopic mechanical properties of Inada granite, some MFT tests were carried out. Fig.3 shows an image of loading state of MFT test, and Fig.4 shows MFT specimen with standard dimensions. The MFT test was performed by applying load by diamond pin to MFT specimen, and the Mode I fracture toughness K_{IC} is estimated from maximum load P_{max} using the following equation. (Tada et al., 1973).

$$K_{IC} = \frac{6P_{max}S\sqrt{\pi a}}{W^2B}F\left(\frac{a}{W}\right) \quad (1)$$

Where a is depth of the notch, W is thickness of the specimen, B is width of the specimen, S is distance between the loading point and the notch, and F is function of dimensionless notch length a/W.

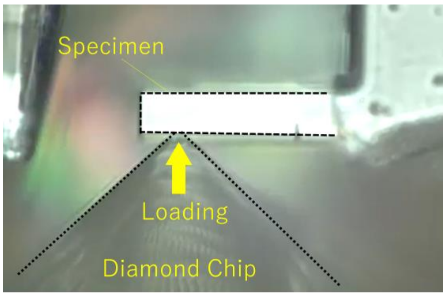


Fig.3 Loading state of MFT test.

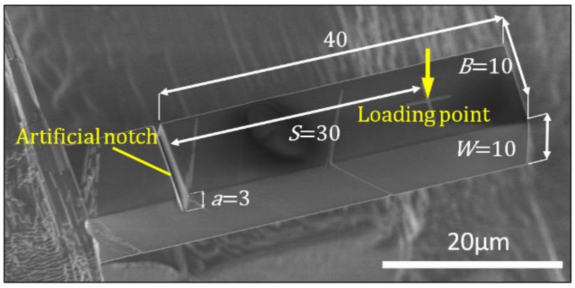
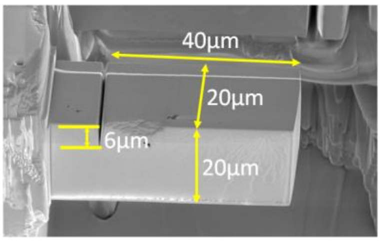
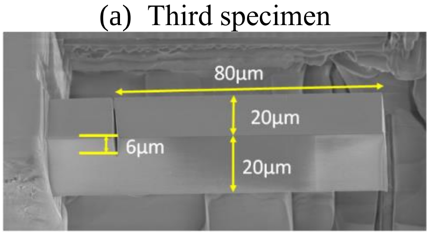


Fig.4 SEM images of MFT specimen with standard dimensions.

In this study, four composed minerals in Inada granite; quartz, plagioclase, K-feldspar and biotite, and three boundaries in; plagioclase and K-feldspar, quartz and plagioclase, quartz and K-feldspar, were the targets of MFT tests. In addition, especially mineral grains, MFT tests were also carried out using two different dimension specimens to investigate the size effect of MFT. Fig.5 shows different dimension specimens.



(a) Third specimen



(b) Forth specimen

Fig.5 SEM images of different dimension specimens; (a)third specimen, (b) forth specimen.

Fig.6 shows all the results of the MFT tests. In mineral grain specimens, The MFT values of mineral grains show that the MFT of quartz was the largest value, and biotite was the smallest value, plagioclase and K-feldspar were medium. And the size effect in MFT didn't appear. In the grain boundaries, the MFT value decreased from the respective minerals' MFT value composing boundaries.

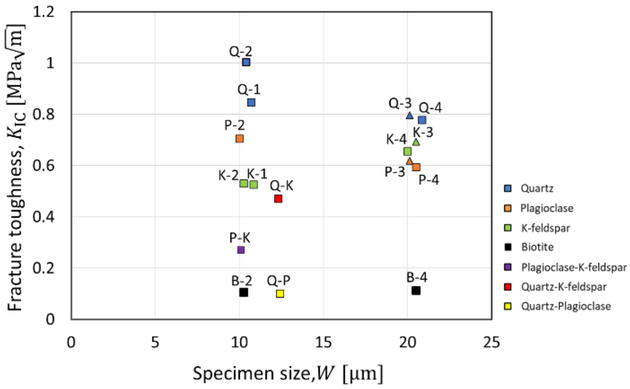


Fig.6 All the results of MFT tests, and relation between K_{IC} and specimen size

4.FRACTURE PROCESS SIMULATION BASED ON MEASUREMENTS OF MFT

Based on the mechanical properties of microscopic mineral grains and grain boundaries measured in MFT tests, a numerical SCB simulation was generated.

In this study, Bonded-Particle model (BPM), as known as a type of discrete element method (DEM), was used in PFC 2D, which can be implemented two-dimensional codes.

In the BPM simulation, a rock is considered as an assemblage of particles bonded at their contact points, and cracking is simulated as the bond breakage. therefore, the microparameters determined the bonding state were important factors in BPM

First, simulated MFT tests, microparameters (mainly tensile strength σ, cohesion c, Young's modulus E) in respective minerals and boundaries were calibrated using K_{IC}, specimen dimensions, and load-displacement curve obtained from MFT tests. Calibrated microparameters are listed in Table.1.

Table.1 Calibrated microparameters

Mineral grains	Values of microparameters σ [MPa]	C [MPa]	E [GPa]
Quartz	23.5	23.5	18.6
Plagioclase	17.2	17.2	17.5
K-feldspar	15.7	15.7	26.0
Biotite	2.8	2.8	2.5
Grain boundaries	σ [MPa]	C [MPa]	k [10^{13}×N/m^3]
Plagioclase/K-feldspar	0.90	5.3	10.0
Quartz/K-feldspar	1.8	9.0	8.0
Quartz/Plagioclase	0.75	3.2	40.0

Next, the numerical SCB simulation applying calibrated microparameters was generated. In this study, the numerical SCB model was contained from microstructure such as mineral grains and grain boundaries. Fig.7 shows an example of the SCB model with 32mm radius. To compare with laboratory SCB tests, and verify the size effect, the SCB models with different radius were also simulated.

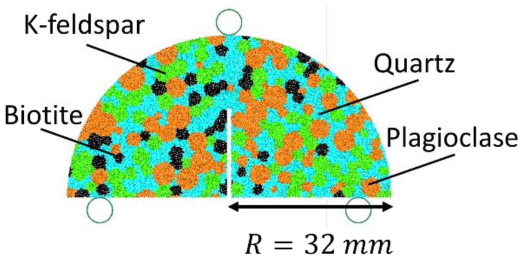


Fig.7 An example of numerical SCB model with radius 32mm

The simulated K_{IC} values with respective radius are summarized in Table.2, and compared with laboratory tests' K_{IC}. The simulation results are in good agreement with those obtained from the laboratory tests, and reproduced their size effect.

Table.2 Simulated K_{IC} values compared with laboratory test

Radius [mm]	25.8	32	80
Laboratory test, K_{IC} [MPa$\sqrt{\text{m}}$]	0.87	0.96	1.11
Numerical simulation, K_{IC} [MPa$\sqrt{\text{m}}$]	0.81	0.89	1.30

5. DISCUSSION

In BPM simulation, microparameters generally are calibrated by using laboratory test results such as tensile and compression tests. Therefore, the numerical SCB simulation was performed using the microparameters applied in previous study (Peng et al., 2018). The K_{IC} results in the conventional method are much larger than the laboratory test results. It indicates that calibration based on MFT tests is valuable for generating fracture process simulations.

In this study, the following fracture process was observed in numerical SCB simulation. First, due to its weak fracture toughness, boundary bonds near the notch were broken and those cracks were propagated. Next, intragranular (inside grains) bonds were broken. Finally, grain fracture and boundary fracture were combined to produce macro fracture.

Those fracture process is considered to reproduce the fracture mechanism in the laboratory test. Some previous studies on SCB tests (Guo et al., 2021) showed similar phenomenon which was investigated by using acoustic emission (AE): first, a number of AE events are distributed in a fan shape in front of notch tip, and as the load increases, more AE events are concentrated in the fracture path. This indicates that the micro cracking process in the numerical SCB simulation corresponds to observation of AE events.

The proposed numerical SCB model reproduced the size effect in K_{IC}. Fig.8 shows the comparison of K_{IC} values between the proposed numerical SCB model and the quartz SCB model, which only contained from quartz microparameters. As the specimen radius increases, the K_{IC} value with GBM is approaches the K_{IC} with quartz. Thus, the size effect is considered to be affected by presence of quartz. Fig.9 shows the bonding state just after the peak load. In the simulation of this study. The cracks mainly propagated in the boundaries. However, if there are no grain boundaries in the fracture path, the cracks are forced to propagate inside grains. There is the possibility of presence of quartz in the fracture path increases and the fracture toughness also increases, as the specimen radius increases.

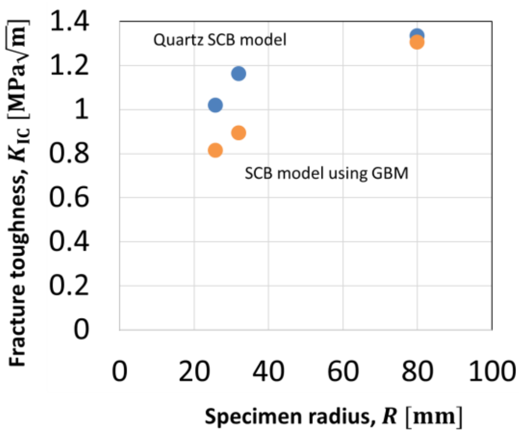


Fig.8 Comparison between quartz SCB model and GBM SCB model.

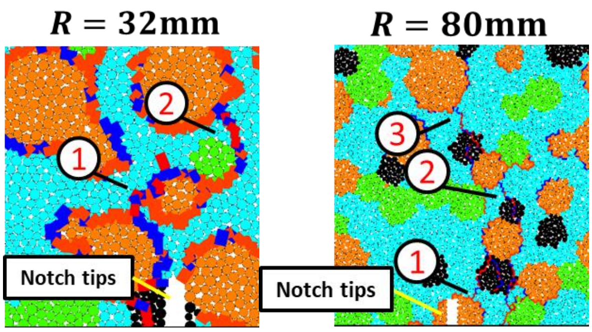


Fig.9 Bonding state just after peak load

Some studies show the relationship between fracture toughness and grain size. Generally, two characteristics are observed: as the grain size decreases, the fracture toughness increases and the number of boundary cracks also increases (Guo et al., 2020). Carrying out the numerical simulation using fine-grained SCB model, which contained from half the grain size compared to the standard SCB model, the characteristic of fracture process reproduced to previous study: the number of boundaries and bond breakage increased. However, in fine-grained SCB model, fracture toughness decreased, because of decreasing of grain size. This was attributed to the increased number of weak boundaries. In addition, those results suggested that different grain sized rocks may have different mechanical strength such as fracture toughness.

6. CONCLUSIONS

In this study, the fracture process simulation of Inada granite was generated, in order to investigate the fracture mechanism of rocks from macroscopic and microscopic aspects. For this purpose, the SCB test, which measures the macroscopic fracture toughness, and MFT test, which measures the microscopic fracture toughness, was carried out. The main concluding remarks are as following:

1) The macroscopic fracture toughness of the Inada granite was measured by SCB test and the size effect was verified.

2) The microscopic fracture toughness (MFT) values of minerals of the Inada granite (quartz, potassium feldspar, plagioclase and biotite) were measured by MFT tests. MFT showed no size effects.

3)The MFT values of grain boundaries were measured. These showed lower MFT than the mineral grains.

4) The numerical SCB simulation model was generated based on measuring MFT tests results. It reproduced the laboratory test results well and showed size effects. And, it showed that fractures preferentially occurred at grain boundaries.

5)The size effect of fracture toughness was concluded to be due to the increasing number of quartz present in the fracture path, as the specimen radius increases.

6)The intergranular cracks increased with decreasing grain size in the numerical simulation. And the possibility that rocks with different grain size may have different intergranular mechanical strength was suggested.

7.REFERENCES

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