International Journal of Rock Mechanics & Mining Sciences 85 (2016) 119–128

Contents lists available at ScienceDirect

International Journal of
Rock Mechanics & Mining Sciences

journal homepage: www.elsevier.com/locate/ijrmms

Discrete element modeling of the process zone shape in mode I fracture at peak load and in post-peak regime

Ali Fakhimi*, Fang Wan

Department of Mineral Engineering, New Mexico Institute of Mining and Technology, Socorro, NM 87801, USA

ARTICLE INFO

Article history:
Received 27 November 2015
Received in revised form
6 March 2016
Accepted 21 March 2016
Available online 31 March 2016

Keywords:
Shape of fracture process zone
Discrete element modeling
Size effect
Post-peak deformation
Servo-controlled loading

ABSTRACT

The bonded particle discrete element method is used to study the fracture process zone in three point bending tests of notched beams. Five different specimen sizes and different material ductility are studied. To capture the damaged contacts around the induced macro-crack (fully softened and detached contacts in front of the notch), a contact bond model with softening is implemented. Material ductility is modified by changing the post-peak slope of the load-displacement curve of the contact points between the particles. A servo-controlled loading routine is defined to capture the post-peak behavior and to reveal the impact of macro-crack extension on the size of the process zone. The results show that with the increase in the specimen size, both the width and length of the fracture process zone increase. Examination of the orientation of the contacts around the macro-crack suggests that while close to the macro-crack, contacts with a wide orientation range enter into the softening regime, damaged contacts at some horizontal distance from the induced vertical macro-crack have preferential directions; the damaged contacts are parallel or sub-parallel to the macro-crack at some distance from the macro-crack.

1. Introduction

In fracture of quasi-brittle materials around a crack or notch tip, a non-linear zone called fracture process zone (FPZ) is developed. This zone which consists of many micro-cracks and damage points affects the fracture toughness and the energy consumption in the process of creating new crack surfaces. The presence of FPZ can alter the fracture load of a structure and may help to stabilize the crack propagation compared to a situation that a purely linear elastic fracture mechanics (LEFM) is applicable. Furthermore, the existence and size of FPZ can modify the size effect and post-peak behavior of a material. Therefore, characterization of FPZ is important in studying the mechanical behavior of quasi-brittle materials.

Fracture process zone has been studied both experimentally and numerically in the literature. For the physical studies, acoustic emission (AE) method, DIC (digital image correlation), and X-ray techniques have been employed. Otsuka and Date[1] studied the FPZ around notch tips of concrete specimens in mode I loading using the AE and X-ray techniques. Specimens with different sizes were used. Their results suggest that the size of FPZ changes with specimen size. Particularly, their measurements of the FPZ length and width indicate that the length of FPZ grows faster than the width of the FPZ as the specimen size increases; the shape of process zone is affected by the specimen size. Li and Marasteanu[2] conducted semi-circular bend tests on specimens made of several asphalt mixtures. AE was employed to capture the evolution and size of FPZ around the notch tip. In their study, the FPZ at the peak load was defined as a rectangular zone (with one side of the rectangle positioned at the notch tip) that included the AE events corresponding to 95% AE energy. Comparison of their results showed that the size of FPZ was significantly affected by the aggregate type and the porosity of the material. Furthermore, they observed that while the length of the initial notch had no noticeable influence on the width of the FPZ, increase in the notch length significantly reduced the length of FPZ. Sandstone specimens were tested in three-point bending in Ref. 3, and the FPZ size was studied using the AE technique. The authors concluded that for the specimen sizes they studied, the size and particularly the width of the FPZ may be considered as a material property related to grain size and porosity. Zhang and Wu[4] performed three-point bending tests on concrete specimens and studied the FPZ by detecting the AE events. They concluded that the length of the FPZ is greatly affected by the specimen size and it cannot be considered as a material property. They also showed that the length of the FPZ reduced as the crack approached the specimen boundary.

Numerical and theoretical studies have been performed in studying the FPZ as well. Bazant and Kazemi[5] used a theoretical argument to show that the length of the FPZ changes with the specimen size, but it eventually approaches to its asymptotic value

---

* Corresponding author.
E-mail address: hamed@nmt.edu (A. Fakhimi).

http://dx.doi.org/10.1016/j.ijrmms.2016.03.014
1365-1609/© 2016 Elsevier Ltd. All rights reserved.

for very large specimens. This asymptotic value of the FPZ length was considered as a material property. Fakhimi and Tarokh[6] showed both theoretically and numerically that there is size effect on the size of FPZ and that only for large specimens, the length and width of the FPZ may be considered as intrinsic material properties. Elias and Bazant[7] applied the lattice-particle numerical model to study the FPZ. They concluded that smaller specimen sizes and those with deeper notch resulted in narrower FPZ. Haidar et al.[8] performed both physical and numerical bending tests on notched specimens of a model material and tried to obtain a correlation between the internal length in the nonlocal constitutive relations and the width of the FPZ. In their study, they noted that increase in porosity resulted in more ductile material behavior and increase in the width of the FPZ; the process zone size is affected by the material ductility. Bonded particle model was utilized in Ref. 9 in simulation of FPZ in three point bending tests. They noticed that the specimen size can affect both the width and length of the FPZ. Furthermore, the shape of FPZ, defined as the ratio of its length to its width, changes by increase in the specimen size.

While the efforts in the literature in characterizing the FPZ in quasi-brittle materials are of great importance and have identified some key aspects of FPZ, more work is needed for further clarification of the effect of specimen size on the shape of FPZ. Particularly, it appears that there is a lack of effort in studying the FPZ in the post peak regime. This is perhaps due to the difficulty in controlling the stability of the physical and numerical testing, particularly when class II rock behavior is encountered.[10]

In this paper, a bonded particle discrete element system and three point bending tests are used to investigate the effect of specimen size and material ductility on the size and shape of the FPZ. The FPZ is studied at both the peak load and in the post-peak regime. The post-peak behavior of the simulated rock is captured by introducing a servo-controlled loading system. The servo-controlled loading system helps to prevent violent failure of the specimen in the post-peak regime.

2. Discrete element model

The numerical analysis was conducted using the CA2 computer program.[11,12] The rock was modeled as a bonded particle system. In the bonded particle discrete system, the circular particles interact with each other with normal and shear springs at the contact points. The normal and shear spring constants (k_n and k_s) are to simulate the rock elasticity. The friction coefficient (μ), and normal and shear bond values (n_b and s_b) are needed as well for interaction of the particles and to assure that the simulated rock can withstand the applied deviatoric stresses. In addition to these micro-mechanical parameters, the genesis pressure (σ_0) which is the applied pressure during the sample preparation is required to induce a small initial overlap of the particles. It has been shown that this initial overlap can help to more realistically calibrate the bonded particle system to mimic the rock mechanical behavior.[11] To capture the process zone around the notch tip, a tensile softening contact bond model was implemented. In this model, if the contact force between two particles exceeds the normal bond strength (n_b), the contact strength is allowed to linearly reduce with further extension of the contact. The slope of the softening line is called k_{np} in this paper. Fig. 1a shows normal contact force vs. the contact separation. Note that by increasing the post-peak slope in Fig. 1a, more brittle rock behavior can be modeled in mode I fracture. The shear contact force vs. the shear contact displacement is shown in Fig. 1b. For the shear force, no gradual softening was implemented as only the mode I fracture was studied in this paper and the numerical analysis suggested that no actual shear micro-cracks were developed.

The numerical model was calibrated to follow the mechanical behavior of Berea sandstone. The sandstone has an elastic modulus of 14 GPa, a Poisson's ratio of 0.32, a uniaxial compressive strength (q_u) of 55–60 MPa, and a bending tensile strength (for a 80 mm × 240 mm beam) of 8.6 MPa. The calibration procedure was conducted using the technique introduced by Fakhimi and Villegas[13] and resulted in the following model properties: $k_n = 22.0$ GPa, $k_s = 5.5$ GPa, $n_b = 2800$ N/m, $s_b = 12300$ N/m, $\mu = 0.5$, $\sigma_0 = 2.2$ GPa, and $k_{np} = 1.83$ GPa ($k_n/k_{np} = 12$). The range of 0.27–0.33 mm ($R_{ave} = 0.3$ mm) was used for the radii of circular particles; the grain size for the Berea sandstone is from 0.1 to 0.8 mm. Note that the particle size in the discrete element method affects the fracture toughness and the size of the fracture process zone and therefore, particle size in the simulation must be chosen to be consistent with the grain size of the rock.[14] This requirement is particularly more important when the rock grains are much stronger than the grains contact points and hence grains remain mostly intact during the rock fracture.

The simulated material with the above micro-parameters was tested in uniaxial compression (40 mm × 80 mm specimen) and three-point bending (80 mm × 240 mm specimen) to verify the accuracy of the calibration procedure. As correctly explained in Ref. 15, a 2D bonded particle model is neither plane stress nor plane strain, since the deformation in the third direction is not considered in solving the governing equations. Therefore, depending on the actual physical problem, the simulation outputs must be interpreted as the plane stress or plane strain results. The three point bending tests were performed assuming a plane stress situation. The elastic modulus and Poisson's ratio were obtained by performing a numerical uniaxial compression test on a

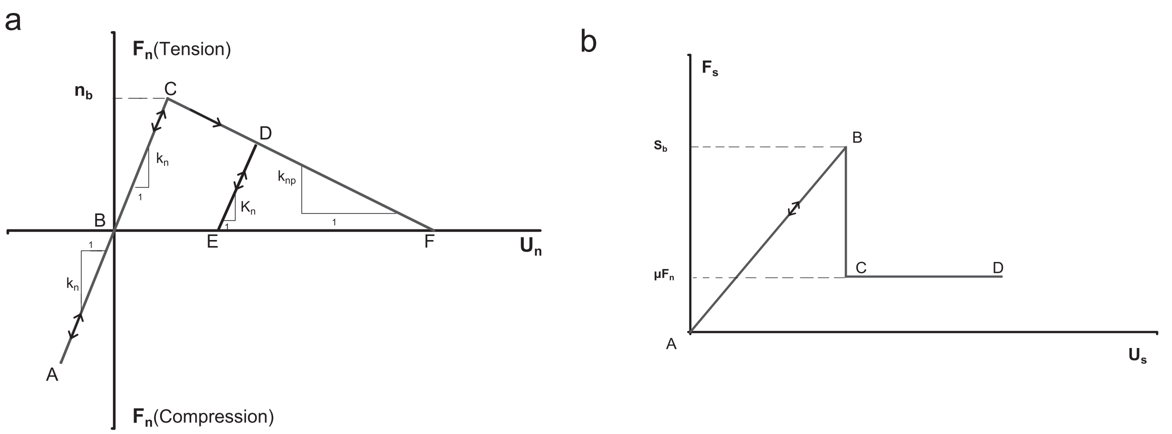

Fig. 1. The relationship between (a) normal contact force and normal contact displacement, (b) shear contact force and shear contact displacement.