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Modeling wave propagation induced fracture in rock with correlated lattice bond cell

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ABSTRACT

The correlated lattice bond cell model (CLBC) is used to account for the characteristics of the mesostructure of rock. Each mineral grain is modeled as a discrete unit bond cell. A linear modified Stillinger–Weber potential is adopted to characterize the unit bond cell. By this method, the lattice model can not only represent the variable Poisson ratio, but can also simulate more complex fracture behaviors than the two-body interaction-based lattice model. It can precisely simulate the stress wave propagation in rock with different Poisson ratios. With a simple bond rupture criterion, the spalling fracture induced by stress wave is well simulated. To represent the heterogeneity of rock, the moduli of bond cells are assumed to be random, following a Weibull distribution. The simulation results demonstrate that the distinct spalling fracture is likely to initiate in a hard rock subjected to impact load, but not in a soft rock. The heterogeneity has little effect on the spalling fracture.

1. Introduction

The stress wave propagation can induce fracture in rock, leading to many geological disasters. However, the existed mechanical models are still inadequate to effectively simulate this phenomenon. The continuum mechanics-based method is the most popular approach to this problem by far, but it has many limitations in modeling stress wave-induced fracture. The fracture behaviors, such as initiation, propagation, branching and arresting, cannot be simulated unless a suitable fracture criterion is given in prior. However, the fracture criterion, especially that of the unstable dynamic fracture, is very difficult to provide.

The lattice method pioneered by Hrennikoff[1] provides an efficient approach to the simulation of dynamic fracture. For the lattice method represents a continuum with a discrete bond system, it simulates the continuum fracture process by the successive bond ruptures with a simple bond rupture criterion. The bond rupture criterion is much easier to establish than the fracture criterion of 3D continuum. In the early version of this method, the discrete structure was composed of springs.[2,3] Because the spring only accounts for the normal interaction of two particles, the Poisson ratio it presents is fixed, namely 0.25 for 3D case and 1/3 for 2D case. This restricts its application to a wider range of materials. To address this problem, the beam was introduced into the particle system to replace the spring.[4,5] However, in the beam system the particle rotation, an additional degree of freedom to the particle displacement, was introduced. To represent the variable Poisson ratio only in terms of particle displacement, Zhao et al.[6] developed the distinct lattice spring model. In this method, the normal and the shear deformation of spring are separately accounted for. However, the shear deformation of spring directly computed by the particle displacement includes the rigid body rotation. To exclude the rigid body rotation, a local strain-based method was adopted in.[6] In order to account for the bond rotation effect, Wang et al.[7,8] introduced the angular spring to the lattice model. By this method, the variable Poisson ratio can be represented. These advances of lattice method make the fracture simulation more efficient. However, in the lattice method, the bond parameter calibration is case-dependent. Different topological structure of unit cell leads to different micro–macro parameter relationship. This makes it difficult to calibrate the bond parameters of 3D lattice model. Moreover, the conventional lattice model is incapable of presenting the characteristics of mesostructure of rock, which consists of mineral grains on mesoscale.

To develop a lattice model that can represent the characteristics of mesostructure of rock, Zhang[9] developed the discretized virtual internal bond method (VIB) based on the VIB theory.[10] The discrete structure of discretized-VIB consists of unit bond cells. Each unit bond cell can have any geometry with any number of bonds. A universal bond parameter calibration method was

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proposed based on the ideal unit cell conception.[9] The discretized-VIB employs the two-body potential to characterize the bond energy. The two-body potential only accounts for the normal interaction between two particles, missing the effect of bond rotation. Therefore, the discretized-VIB presents a fixed Poisson ratio. Furthermore, from the standpoint of fracture mechanism, the two-body potential indicates that the fracture initiation and propagation only result from the normal separation of two particles, irrelevant to the shear effect between particles. Therefore, the two-body potential is too simple to simulate more complex fracture behaviors. Instead, the Stillinger–Weber (SW) potential[11] indicates that the fracture initiation is not only related to the normal deformation of bond, but also related to the bond angles. Though SW potential is specially developed for the silicon material, the fracture mechanism it represents is applicable to other materials. Zhang et al.[12] modified the SW potential and extended it to other materials than silicon. To address the fixed Poisson ratio problem of the discretized-VIB, Zhang and Chen[13] adopted the modified SW potential to describe the unit bond cell. For the bonds in a unit cell are correlated together by the SW potential, the discretized-VIB employing the SW potential is also called the correlated lattice bond cell model (CLBC). Since a more elaborate fracture mechanism is incorporated, the CLBC can capture more characteristics of dynamic fracture.

Rock is a kind of heterogeneous quasi-brittle material. To develop a suitable lattice model for rock based on CLBC, we use the linear modified SW potential to describe the unit cell of rock and introduce the heterogeneity on the mineral grain level. With this model, we simulate the stress wave propagation in rock with variable Poisson ratios and the induced spalling fracture. The aim of the present work is to provide a simple and efficient lattice method to simulate the stress wave-induced fracture in rock.

2. Modeling rock with correlated lattice bond cells

2.1. Brief introduction to Stillinger–Weber potential and its modified version

The SW potential[11] was originally proposed to simulate the silicon material in molecular dynamics methodology. It takes the form

$$\Phi = \sum_{i<j} \Phi_2(r_{ij}) + \sum_{\substack{i\neq j \\ j<k}} \Phi_3(r_{ij}, r_{ik}, \theta_{ijk}) \tag{1}$$

where Φ_2, Φ_3 stands for the two- and three-body interaction, respectively; r_{ij} the bond length of bond vector $\mathbf{r}_{ij}$; θ_{jik} the bond angle subtended by the bond vector $\mathbf{r}_{ij}, \mathbf{r}_{ik}$ at vertex i. The specific expressions of Φ_2 and Φ_3 are.

$$\Phi_2(r_{ij}) = A\left[B\left(\frac{\ell_0}{r_{ij}}\right)^p - \left(\frac{\ell_0}{r_{ij}}\right)^q\right]\exp\left(\frac{1}{r_{ij}/\ell_0 - r_0^*}\right)$$

$$\Phi_3(r_{ij}, r_{ik}, \theta_{jik}) = \lambda\left(\cos\theta_{jik} + \frac{1}{3}\right)^2 \exp\left(\frac{\gamma}{r_{ij}/\ell_0 - r_0^*}\right)\exp\left(\frac{\gamma}{r_{ik}/\ell_0 - r_0^*}\right) \tag{2}$$

in which r_0^* is the cutoff radii; the 1/3 being the minus cosine of the"ideal' tetrahedral angle; ℓ_0 is the bond length when undeformed. The parameters A and λ implicitly contain the energy scaling parameter $\varepsilon$of the original two- and three-body interactions in Ref. 11.

Eq. (2) indicates that the bond energy is not only related to the normal deformation of itself, but also related to the bond angles subtended with other bonds. This equation is especially applicable to the silicon materials because the three-body interaction takes the 'ideal' tetrahedral angle as the reference value of bond angle in the current configuration. Such three-body interaction tends to arrange the randomly distributed bonds into an 'ideal' tetrahedral structure. Thus, the original SW potential is only applicable to the silicon material, not to others. In Ref. 12, the SW potential was modified in such manner that the bond angle in the reference configuration, not the 'ideal' tetrahedral angle, was taken as the reference value of bond angle in the current configuration. The modified SW potential[12] is

$$\Phi_2(\tilde{r}_I) = A\left(B\tilde{r}_I^{-p} - \tilde{r}_I^{-q}\right)\exp\left[\left(\tilde{r}_I - r_0^*\right)^{-1}\right]$$

$$\Phi_3(\tilde{r}_I, \tilde{r}_J, \theta_{IJ}) = \lambda\left(\cos\theta_{IJ} - \cos\theta_{IJ0}\right)^2 \exp\left[\gamma\left(\tilde{r}_I - r_0^*\right)^{-1} + \gamma\left(\tilde{r}_J - r_0^*\right)^{-1}\right] \tag{3}$$

in which $\tilde{r}_I, \tilde{r}_J$ are the normalized bond length, $\tilde{r}_I = r_{ij}/\ell_0$, $\tilde{r}_J = r_{ik}/\ell_0$; θ_{IJ0} stands for the bond angle subtended by the bond $\mathbf{r}_{ij}$ and $\mathbf{r}_{ik}$ in the reference configuration whereas θ_{IJ} its value in the current configuration.

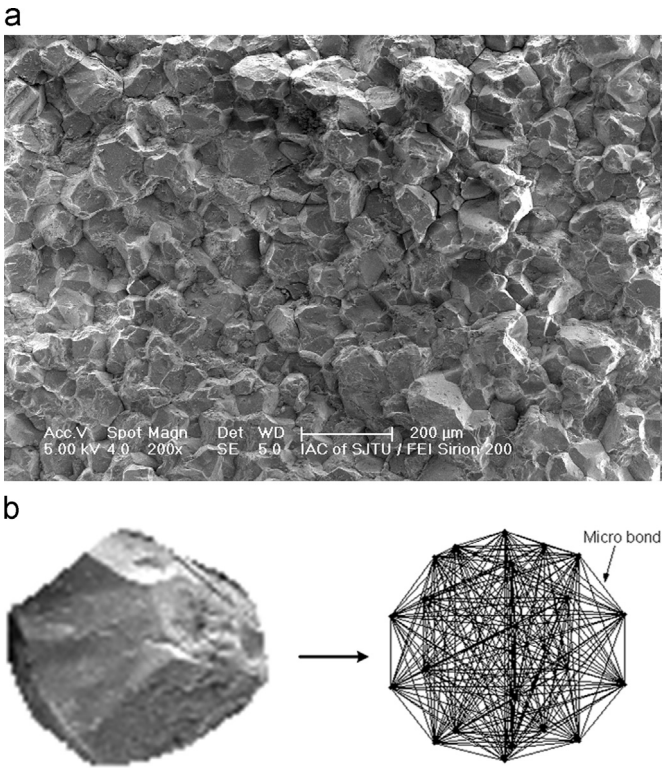

Fig. 1. Modeling rock with correlated lattice bond cells (a) the mesostructure of rock (SEM image of marble) consisting of mineral grains; and (b) a continuous mineral grain is modeled as a discrete unit bond cell.

2.2. Modeling mineral grain with correlated lattice bond cells

The mesostructure of rock is shown in Fig. 1a, which consists of mineral grains on the mesoscale. Originally, the mineral grain is a continuum. In the present method, it is modeled as a discrete system, i.e., a correlated lattice bond cell (Fig.1b). Considering that rock is a typical elastic-brittle material, the energy of a unit bond cell is characterized by the linear modified SW potential.

$$\Phi_2 = \frac{1}{2}A\ell_0^2(\tilde{r}_I - 1)^2$$

$$\Phi_3 = \frac{1}{2}\lambda(\theta_{IJ} - \theta_{IJ0})^2 \tag{4}$$