Chapter 8
Estimation of Energy of Fracture Initiation in Brittle Materials with Cracks

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Abstract We study deformation and fracture of a brittle material under mixed quasi-static loading. Numerical simulations of deformation of a cubic sample containing a single crack are carried out using the particle dynamics method. Effect of ratio of compressive and shear loads on energy of fracture initiation is investigated for two crack shapes and various crack orientations. The energy of fracture initiation in a material containing multiple cracks is estimated using the non-interaction approximation. It is shown that in the case of mixed loading (compression and shear) the energy is significantly lower than in the case of pure compression. Presented results may serve for minimization of energy consumption during disintegration of solid minerals.

Keywords: Brittle fracture · Fracture initiation · Cracks · Particle dynamics method · Desintegration of rocks · Energy consumption

8.1 Introduction

One of the key technological challenges for mining industry is minimization of energy consumption during disintegration (fracture) of solid minerals (Vaisberg and

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H. Altenbach and A. Öchsner (eds.), *State of the Art and Future Trends in Material Modeling*, Advanced Structured Materials 100,
https://doi.org/10.1007/978-3-030-30355-6_8

Kameneva, 2014; Vaisberg et al, 2018a,b). The energy required for fracture of rocks strongly depends on their heterogeneous internal structure. Development of scanning technologies, for example, computer microtomography, makes it possible to determine shapes and sizes of heterogeneities (Vaisberg and Kameneva, 2014; Vaisberg et al, 2018a; Vesga et al, 2008). However, finding relation between microstructure of a rock and its mechanical properties is still a challenging problem for mechanics (Kachanov and Sevostianov, 2018; Altenbach and Sadowski, 2015; Altenbach and Öchsner, 2011).

Influence of heterogeneities on effective elastic properties of materials is studied in many works on micromechanics (Torquato, 1991). Materials with pores (Shafiro and Kachanov, 1997; Kumar and Han, 2005; Bîrsan and Altenbach, 2011), cracks (Sayers and Kachanov, 1991; Saenger, 2008; Min and Jing, 2003; Grechka and Kachanov, 2006), and inclusions (Shafiro and Kachanov, 2000) of different shapes are considered. Proper microstructural parameters determining contribution of heterogeneities to effective properties are introduced (Kachanov and Sevostianov, 2005; Kachanov, 1999). State of the art in calculation of effective elastic properties is summarized in the recent book (Kachanov and Sevostianov, 2018). In particular, the non-interaction approximation allowing to calculate effective properties analytically is discussed in detail.

Success of micromechanics in prediction of effective elastic properties is caused by the fact that these properties are insensitive to many features of real microstructure. Estimation of influence of heterogeneities, e.g. cracks, on strength properties is more challenging. Complexity of estimation of strength properties is related to the fact that strength is determined by local stress fields. Therefore many works are devoted to development of numerical schemes for accurate calculation of the local fields (Linkov, 2002; Krivtsov, 2007; Kuna, 2013). In particular, efficient methods for calculation of stress intensity factors in materials containing multiple cracks are proposed in Rejwer et al (2014); Kushch et al (2009); Jaworski et al (2016). Relation between distribution of stress intensity factor and effective strength of a material is discussed in Rejwer et al (2014).

From practical point of view, it is important to find relation between loading type and energy required for fracture of a material. This problem is not fully covered in literature. In Bratov and Krivtsov (2016), a simple two-dimensional model for estimation of energy of fracture initiation is proposed. Influence of loading type on the energy is investigated. It is shown that mixed loading (compression and shear) is energetically more efficient than pure compression. In the present paper, we generalize the results of Bratov and Krivtsov (2016) for the three-dimensional case.

The paper is organized as follows. In Sect. 8.2, discrete model of a brittle material is presented. In Sect. 8.3, simulation of deformation and fracture of a sample containing an infinite rectangular crack is carried out. Energy of fracture initiation under various loads for different crack orientations is calculated. Numerical results are compared with analytical estimates (Bratov and Krivtsov, 2016). In Sect. 8.4, the energy of fracture initiation is calculated for a penny-shaped crack. Generalization for the case of multiple non-interacting penny-shaped cracks is carried out in Sect. 8.5.

8.2 Discrete Model of a Brittle Material

In this section, a discrete model of deformation and fracture of a brittle material (e.g. rock) is presented. A material is simulated using the particle dynamics method (Krivtsov, 2007, 2004, 2003). In this method, a material is represented as a set of interacting particles (~material points) connected by bonds. Cubic sample of a material is considered. Number of particles in the sample is of order of $5 \cdot 10^5$. Particles form a quasi-random lattice (Tsaplin and Kuzkin, 2017). Positions of the particles are calculated using the following algorithm, proposed in Tsaplin and Kuzkin (2017). A perfect face-centered cubic lattice (FCC) is created. Particles are located at nodes of the lattice (Fig. 8.1A). Then particles get random displacements (Fig. 8.1B). Magnitudes of the displacements are of order of $0.4d$. Here d is the step of the FCC lattice. Each pair of particles at the distance less than $1.9d$ is connected by a linear elastic spring (bond). On average, each particle has 20 bonds. The equilibrium bond length is equal to the initial distance between connected particles. In Tsaplin and Kuzkin (2017) it is shown that resulting material has isotropic elastic and strength properties.

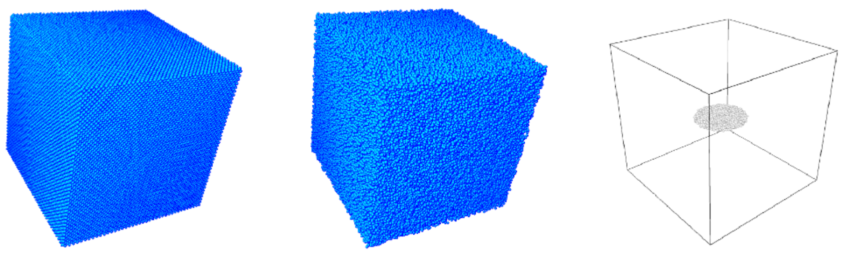
During the simulation, the following equations of motion for particles are solved numerically:

$$m\dot{\mathbf{v}}_i = \sum_j \mathbf{F}_{ij} - \beta \mathbf{v}_i. \tag{8.1}$$

Here, summation is carried out over all particles j connected with particle i; m is particle mass; $\mathbf{v}_i$ is particle velocity; $\mathbf{F}_{ij}$ is force in the bond connecting particles i and j; β is coefficient of artificial dissipation, which is introduced in order to suppress vibrations caused by deformation of the sample. Forces, $\mathbf{F}_{ij}$, arising in bonds are calculated as

$$\mathbf{F}_{ij} = c_{ij}(r_{ij} - r_{ij}^0)\mathbf{e}_{ij}, \qquad c_{ij} = c_0 \frac{d}{r_{ij}^0}, \tag{8.2}$$

where c_{ij} is bond stiffness; r_{ij} is distance between particles i, j; r_{ij}^0 is initial bond length; $\mathbf{e}_{ij}$ is unit vector directed along the line connecting the particles; c_0 is



(A) (B) (C)

Fig. 8.1 (A) FCC lattice; (B) quasi-random lattice; (C) an example of a crack in the sample (particles near the crack are shown only) stiffness of a bond with initial length equal to d. Equations of motion (8.1) are solved numerically using the symplectic leap-frog integration scheme with time step $2 \cdot 10^{-2} T_*$, where

$$T_* = 2\pi\sqrt{\frac{m}{c_0}}.$$

Periodic boundary conditions in all space directions are used.

Macroscopic elastic moduli of the considered material are calculated in Tsaplin and Kuzkin (2017). It is shown that the Young modulus and the Poisson ratio are related with microparameters as

$$\nu = 0.255, \qquad E = 1.48\frac{c_0}{d}. \tag{8.3}$$

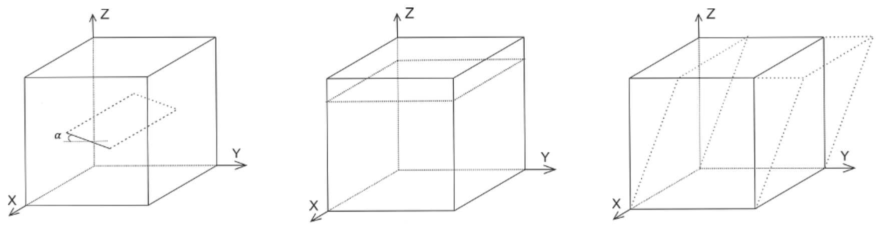
An initial crack is created by removing bonds between the particles that cross a crack surface (Fig. 8.1C). Contact between crack faces is neglected. Crack propagation is simulated by removing bonds, satisfying the following inequality:

$$\frac{r_{ij} - r_{ij}^0}{r_{ij}^0} > \varepsilon_{cr}, \tag{8.4}$$

where ε_{cr} is the critical bond deformation. In further calculations ε_{cr} is equal to $2 \cdot 10^{-4}$.

8.3 An Infinite Rectangular Crack

In this section, we study initiation of fracture (crack propagation) in a sample containing an infinite rectangular crack under various loads. An initial crack is shown in Fig. 8.2A. Angle α is a parameter defining orientation of the crack with respect to direction of loading. Crack length is equal to 0.35 of periodic cell size. During the simulation, every $20T_*$ a periodic cell is subjected to a uniform strain ($\Delta\varepsilon_{zz}$ or $\Delta\varepsilon_{yz}$ or both). Three cases are considered: (a) compression along z axis with increment



(A) (B) (C)

Fig. 8.2 Periodic cell containing an infinite crack (A). Change of the periodic cell under compression (B) and shear (C)

$\Delta\varepsilon_{zz} = 5 \cdot 10^{-6}$ (see Fig. 8.2B); (b) pure shear with increment $\Delta\varepsilon_{yz} = 5 \cdot 10^{-6}$ (Fig. 8.2C) and (c) mixed loading with increments $\Delta\varepsilon_{zz} = \Delta\varepsilon_{yz} = 5 \cdot 10^{-6}$.

Deformation of the sample leads to breakage of bonds. A moment of fracture initiation is tracked by the number of broken bonds. It is assumed that the fracture begins when the number of broken bonds increases by 5% compared to the number of bonds removed for creation of the initial crack. When the criterion is satisfied, the strain energy density is calculated as a sum of potential energies of all bonds in the periodic cell:

$$U = \frac{1}{2V} \sum c_{ij}(r_{ij} - r_{ij}^0)^2, \tag{8.5}$$

where V is volume of the periodic cell. Further U is referred to as the *energy of fracture initiation*.

We compare simulation results with analytical estimates obtained in Bratov and Krivtsov (2016). In Bratov and Krivtsov (2016), a single crack under compression and shear loads applied at infinity is considered in two-dimensional formulation. Solution of corresponding elasticity problem yields stresses near the crack tip. Neuber-Novozhilov fracture criterion (Novozhilov, 1969) is used. The criterion is used for estimation of energy of fracture initiation.

Comparison of analytical estimates Bratov and Krivtsov (2016) with the results of particle dynamics simulations is presented in Fig. 8.3. Every point on the plot corresponds to average over 5 simulations with different realizations of a quasi-random lattice. Figure 8.3 shows that numerical and analytical results are in a qualitative agreement. Deviations are caused by different fracture criteria and material models. In Bratov and Krivtsov (2016), linear fracture mechanics is used. In the framework of this approach, at certain crack orientations the fracture criterion is never satisfied. For example, uniaxial compression of a sample along crack direction does not lead to fracture. Therefore energy of fracture initiation, U, formally tends to infinity (see Fig. 8.3). In contrast, presented discrete model yields finite energy of fracture initiation for any crack orientation. Moreover, fracture is possible even in the absence of a

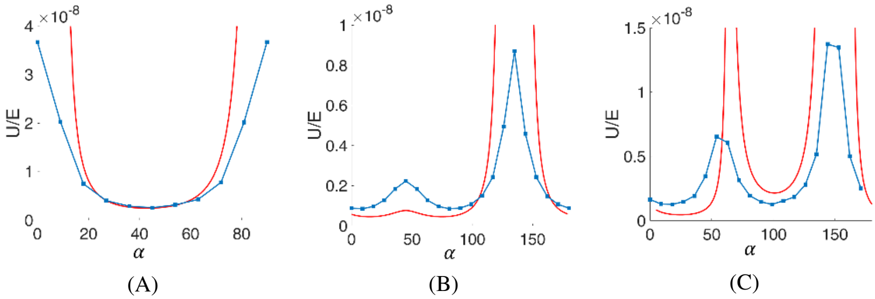


Fig. 8.3 Energy of fracture initiation, U, as a function of rectangular crack orientation under uniaxial compression (A), pure shear (B), and compression with a shear (C). In the latter case $\Delta\varepsilon_{zz} = \Delta\varepsilon_{yz}$. Results of particle dynamics modeling (squares) and analytical estimates (Bratov and Krivtsov, 2016) (solid line) are shown

crack. Additionally, we note that relation between bond breakage criterion (8.4) and the Neuber-Novozhilov criterion is not straightforward.

Figure 8.3 shows that the energy of fracture initiation strongly depends on crack orientation and loading type. In particular, the energy has clear minima corresponding to the most energetically beneficial crack orientations. In the following section, this fact is considered in detail for a penny-shaped crack.

8.4 A Penny-shaped Crack

In this section, initiation of fracture in a sample containing a penny-shaped (circular) crack (Fig. 8.4) is considered. As in the previous section, the sample is subjected to compressive and shear strains with increments $\Delta\varepsilon_{zz}$ and $\Delta\varepsilon_{yz}$ every $20T_*$. Crack orientation is specified by angle α (see Fig. 8.4). The ratio of crack diameter to size of the periodic cell is equal to 0.35.

Influence of crack orientation and ratio of strain increments,

$$k = \frac{\Delta\varepsilon_{yz}}{\Delta\varepsilon_{zz}},$$

on energy of fracture initiation is investigated. Results of numerical simulations are shown in Fig. 8.5. Each point on the plot corresponds to average over 5 realizations of a quasi-random lattice. Figure 8.5 shows that under uniaxial compression ($k = 0$) energy of fracture initiation, U, has minima at $\alpha = 45°; 135°$ and maxima at $\alpha = 0°; 90°; 180°$. Adding shear leads to decrease of minimum and maximum values of fracture initiation energy. Moreover, for $k > 0.5$ and for all crack orientations, the energy of fracture initiation is less than in the case of uniaxial compression. Therefore mixed loading is energetically more efficient than uniaxial compression.

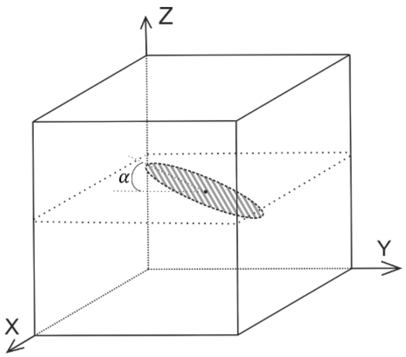


Fig. 8.4 Periodic cell containing a penny-shaped crack

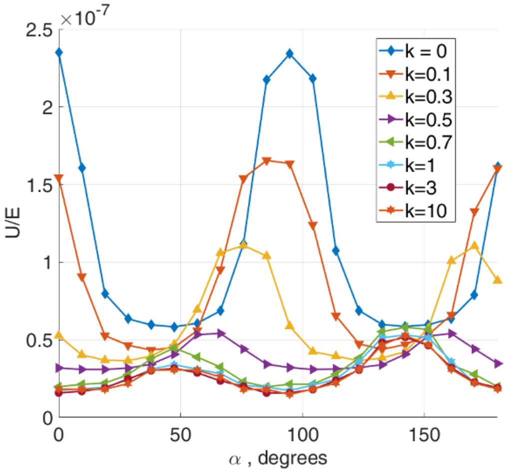


Fig. 8.5 Dependence of the energy of fracture initiation, U, on crack orientation for various ratios of shear and compressive strain increments, k (uniaxial compression corresponds to $k = 0$)

8.5 Multiple Randomly Oriented Penny-shaped Cracks (Non-interaction Approximation)

In this section, energy of fracture initiation in a material containing multiple randomly oriented penny-shaped cracks is estimated using the results obtained above and the non-interaction approximation (Kachanov and Sevostianov, 2018). Consider a material containing randomly located and oriented cracks. Suppose that the cracks are located far from each other. In the framework of the non-interaction approximation, we assume that mutual influence of cracks can be neglected. Then for each crack, the energy of fracture initiation can be estimated using Fig. 8.5. We assume that fracture starts at cracks with orientations, corresponding to minimum of function $U(\alpha)$. For each ratio of shear and compressive strains increments, k, the minima are calculated using results shown in Fig. 8.5. Resulting energy of fracture initiation for a material containing multiple cracks is presented in Fig. 8.6.

Figure 8.6 shows that the energy of fracture initiation has maximum at $k = 0$ (uniaxial compression) and monotonically decreases with increasing shear load. Note that adding a small shear load, significantly decreases energy of fracture initiation. These results are in a good qualitative agreement with experimental observations (Vaisberg et al, 2016) and analytical estimates (Bratov and Krivtsov, 2016).

8.6 Conclusions

Energy of fracture initiation for a material with a single crack under mixed loading (compression and shear) was calculated numerically. Rectangular and penny-shaped cracks were considered. Dependencies of the energy of fracture initiation on crack orientation for various ratios of compression and shear loads were obtained.

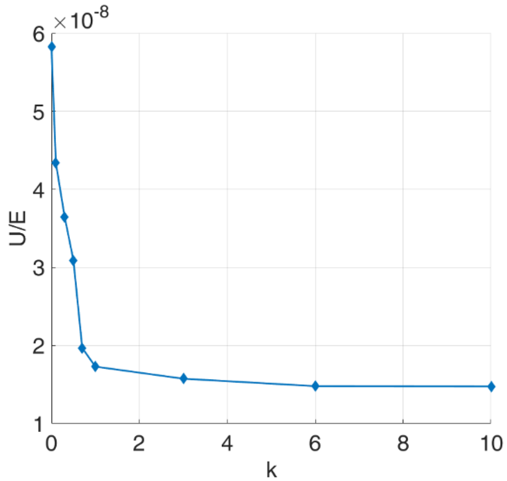


Fig. 8.6 Energy of fracture initiation, U, for a material with multiple cracks as a function of the ratio of shear and compressive strain increments, k

The dependencies were employed for estimation of energy of fracture initiation in a material containing multiple cracks under the non-interaction approximation. It was shown that the energy strongly depends on loading type. It has maximum in the case of uniaxial compression and it decreases monotonically with increasing shear load. It was shown that adding a small shear load yields significant decrease of the energy of fracture initiation.

Presented results may serve for minimization of energy consumption during disintegration of rocks, for example, in vibrational crushers (Vaisberg et al, 2018b). In particular, the results suggest that energy consumption under mixed loading is several times less than under uniaxial compression. This fact is in a good qualitative agreement with experimental observations (Vaisberg et al, 2018b, 2016).

Acknowledgements This work was supported by the Russian Science Foundation (Grant No. 17-79-30056). The authors are deeply grateful L.A Vaisberg for formulation of the problem and useful discussions. The work was initiated in the course of joint investigation of technological processes of vibration disintegration of materials, the main developer of which is REC "Mekhanobr-Tekhnika". Numerical modeling was performed using the Polytechnic supercomputer center at Peter the Great St. Petersburg Polytechnic University.

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