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Comparison of discrete element simulations to theoretical predictions of the elastic moduli of damaged rocks

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ABSTRACT

The influence of damage, represented by a set of micro-cracks, on the elastic parameters of a solid is modeled using the Discrete Element Method (DEM). The results are compared with predictions from damage mechanics theory. In the simulated material, the observed dependence of the elastic parameters on the damage is qualitatively similar to the behavior theoretically predicted for a material containing a collection of micro-cracks which are frictionally sliding under compressive loading and opening under tension. Poisson's ratio of the DEM material is increasing with damage under compression and decreasing with damage under tension. Young's modulus decreases with increasing damage under compression and tension. Under compression the influence of the damage on Poisson's ratio and Young's modulus depends on the coefficient of friction on the crack surfaces, under tension it does not.

1. Background

It has long been known that the mechanical properties of a volume of rock depend not only on its intrinsic material properties but also its "damage", which is generally understood to be some function of the distribution of microcracks within the rock volume. Considering different material properties and loading conditions, a range of theoretical approaches has been developed to describe the effect of the crack density on the elastic parameters such as Young's modulus E, compressibility k, and Poisson's ratio ν, generally following one of two main directions. One group of approaches is based on the treatment of the micro-cracks as elastic inclusions or open cracks.[1–4] The other main group treats the microcracks as sliding surfaces.[5–7] The first group is therefore mainly applicable to situation where the stress is tensile or the compression is small enough so that most of the cracks stay open whereas the second group is more appropriate if the compressive stresses are strong enough to close the majority of the cracks. A combined approach is taking into account open and closed, sliding, cracks simultaneously[8–10] and is therefore applicable to a wide range of stress conditions. Both types of approaches predict a decrease of the elastic moduli (E,k,..) with increasing damage, i.e. crack density. The exact function connecting the damage to the decreasing moduli depends on the details of each specific theory, in particular on the homogenization scheme chosen.[11,4] One fundamental difference between the approaches is that the elastic inclusion approaches predict a decreasing Poisson's ratio with increasing crack density[1,4,12] whereas the sliding crack approach predicts an increase of Poisson's ratio with increasing damage under compression and a decrease under tension.[7] The difference in the behavior between the compressive and tensile regimes is based on the assumption that the cracks will be closed, and therefore sliding frictionally, under compression but open up and behave like a low stiffness elastic inclusion under tension. Furthermore, in the compressive regime, i.e. when the cracks are closed, Walsh [7] also predicts a dependence of the effective elastic parameters of the damaged material on the coefficient of friction μ on the surfaces of the cracks.

However, there is relatively little experimental data available in the published literature which quantitatively describe the relation between a well defined crack distribution and the resulting elastic properties of particular rocks under specific loading situations. While a significant number of studies have been published which are experimentally investigating the elastic behavior of damaged rocks [13–20,9,21,22] not all show data for Poisson's ratio and only few of them (i.e.[16,21,22]) quantify measured crack densities.

The experimental results in triaxial compression tests of Faulkner et al.[16] and Heap et al.[18–20] show a clear increase of Poisson's ratio with increasing damage, thus favoring a "sliding crack" model. In contrast, an estimate of Poisson's ratio based on the velocities of compressive waves (v_p) and shear waves (v_s) published by Inserra er al.[21] suggest that in their experiments Poisson's ratio did decrease with increasing crack density, therefore favoring an open crack/elastic inclusion model. It should also be noted that the experiments by Faulkner et al.[16], showing an increase in ν with damage were carried out at confining stresses of 40–100 MPa. In contrast, observations at ambient pressure show

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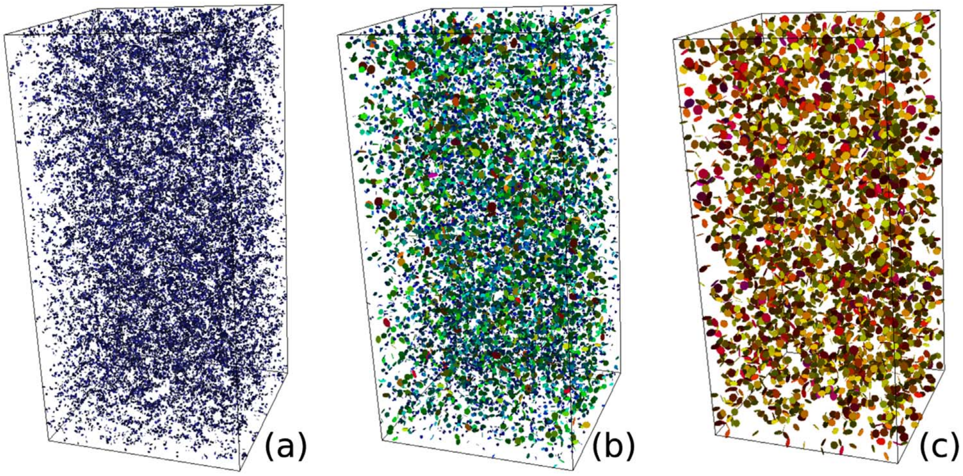

Fig. 1. Different crack distributions with similar damage, i.e. similar total crack area, generated by removing (a) the 31,132 smallest bonds, resulting in $d_2=0.1225$ (b) 11,674 random bonds ($d_2=0.1402$) and (c) the 3891 largest bonds ($d_2=0.1505$). Color shows size of individual micro-cracks.

mixed results. Deformation experiments by Heap et al.[18–20] show an increase of ν with damage whereas the wave speed measurements of Inserra et al.[21] suggest a decrease of ν with damage. This difference can possibly be explained by the different sensitivity of static versus dynamic measurement methods to the opening or sliding of the cracks. Experiments by Schubnel et al.[17] show that the behavior of basalt under increasing pressure is compatible with pressure dependent crack closure and an "elastic inclusion" model without directly measuring crack densities. These experimental results leave the open question which of the two principal approaches is most suitable for the description of damaged rocks under a given set of conditions such as stress and strain rate.

The aim of this study is therefore to present a numerical method capable of capturing the behavior of damaged rocks in a range of loading conditions and to gain a better understanding of the relation between damage and rock elastic properties based on a numerical study using this method. The advantage of this approach is that it allows the arbitrary, controlled variation of the parameters of the crack population representing the damage in the modeled material and the easy observation of the resulting material properties, such as the elastic moduli and the Poisson's ratio.

2. Method

To model the deformation behavior of rocks as brittle-elastic material with a pre-existing distribution of closed micro-cracks sliding under compression we use a discrete element model (DEM) approach.[23–27] This approach has been successfully used to study mechanical behavior of rocks depending on their micro-structure previously[28–31]. A particular advantage of the model is that it is easy to represent a wide range of micro-crack distributions in the model material by removing a given set of particle-particle bonds and replacing them by frictional interactions.

In the DEM approach the material is represented by a large number of spherical particles interacting with their nearest neighbors either through frictional-elastic interactions or through brittle-elastic "bonded" interactions. In order to efficiently run medium to large sized models on current computer hardware the parallel DEM implementation "ESyS-Particle" [32,33] (https://launchpad.net/esys-particle) has been used for the simulations in this paper. For the bonded interactions between the particles the ESyS-Particle software package implements the bond model described in [34]. To specify the elastic and strength parameters of the bonds we are using the "brittle beam" model,[35] where the normal, shear, bending and torsion stiffness of the bonds are determined from Young's modulus E_b and Poisson's ratio ν_b of an assumed bond material or "cement". This approach is very similar to the bonded particle model presented in [36] which is also based on beam theory. A minor difference is that in [36] Young's modulus E_b and shear modulus G_b are used to parametrize the bond elasticity instead of E_b and ν_b. The failure criterion of the bonds is determined from the cohesion C_b and the angle of internal friction ϕ_b of the bond material. However, because all simulations presented in this paper are run in non-fracture regime the details of the failure criterion do not influence the results. In the models used here the bonds are assumed to have a Young's modulus $E_b = 30\,GPa$ and a Poisson's ratio of $\nu_b = 0.3$. In addition to this choice of micro-scale parameters the macroscopic elastic properties of a specific model material are also influenced by the details of the particle packing[28,33], thus making a calibration of the models necessary. In case of the models used here this results in a Young's modulus $E \approx 34\,GPa$ and a Poisson's ratio of $\nu \approx 0.16$ for the DEM material.

For the basic "undamaged" material a fully bonded DEM material, packed by insertion based algorithm [37] is used. Damage is introduced into the material by removing bonds before the deformation test. Removed bonds get replaced by frictional interactions between the particles similar to the approaches taken in [38,28]. The size of the individual micro-cracks is calculated from the assumed radius of removed bond $r_{ij} = (r_i + r_j)/2$ where r_i and r_j are the radii of the particles which were connected by the bond.

Another option would have been to introduce larger scale cracks as pre-defined surfaces before packing the particles as described in [39]. However, this option was not taken because it would have been much more difficult to ensure a non-intersection criterion for the cracks. Also, the resulting roughness of the crack surfaces would have influenced the crack compliance [40] and the effective friction of the cracks, potentially interfering with the observation of the effect of the intrinsic particle friction on the macroscopic elastic properties.

For a subset of the models three different crack populations have been generated by either systematically removing the bonds with the smallest cross section, a set of bonds picked at random, or the bonds with the largest cross sections. Examples with similar total crack area from each of the three sets are shown in Fig. 1. This was done in order to test if the effects of the damage depend on size distribution of the introduced cracks. The total number of cracks removed was chosen in the range of 2.5–30% of the initial number of bonds in the undamaged material. In addition to the