Anisotropic material behavior in dense, cohesive-frictional powders

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Abstract
The goal of this study is to examine the cohesion and the anisotropy in dense, cohesive powders. This is done using a discrete element method (DEM) for the simulation of a bi-axial box deformation. Our approach includes normal (repulsive/cohesive) and tangential forces as well. Reorganization of the contact network leads first to anisotropy and later to shear band formation and softening behavior from the macroscopic point of view. Both cohesion and friction enhance the material strength. An important result is the fact that the macroscopic cohesion can be related to the maximal microscopic attractive force.

Introduction

The material behavior of powders under large deformations is the issue of this study. For cohesive-frictional powders, the discrete element method is a convenient tool to gain insight into the evolution of, e.g., shear localization. Powders, or more general granular media, are typically inhomogeneous, non-linear, disordered, and an-isotropic on a "microscopic" scale [1-3], where microscopic is to be understood as the particle size. The irregular, random packing responds to deformations via an inhomogeneous and an-isotropic stress distribution, accompanied by reorganizations of the contact-network during deformation. An initially isotropic contact network becomes an-isotropic before the structure of the network reaches its limit of stability. Beyond some peak-stress, softening behavior is obtained [2-5], which is typical for an over-consolidated packing. Our work complements recent studies on shear band formation in frictional-cohesive granular media [4-8], for micro- and macro-modeling [9,10], and in various systems [11,12] for different materials.

The Model System

One possibility to gain insight about the material behavior of a granular packing is to perform elementary tests in the laboratory. Here, we chose as alternative the simulation with the discrete element model [4-8,11,12]. The set-up chosen for the numerical "experiment" is the bi-axial box, see Fig. 1, where the left and bottom walls are fixed. Stress- or strain-controlled deformation is applied to the side- and top-walls, respectively. In a typical simulation, the top wall is slowly shifted downwards, while the right wall moves, controlled by a constant stress p, responding on the forces exerted on it by the material in the box. The motion of the top-wall follows a cosine function, in order to allow for a smooth start-up and finish of the motion so that shocks and inertia effects are reduced, however, the shape of the function is arbitrary as long as it is smooth.

Discrete Element Model

The units of powders are particles, which deform under stress. Since the realistic modeling of the deformations of the particles is much too complicated, the interaction force is related to the overlap of two particles, see Fig. 2. In our simplified model, two particles interact if they are in contact, and the force between two particles is decomposed into a normal and a tangential part. For the sake of simplicity, we restrict ourselves to spherical particles here. The normal force is, in the simplest case, a linear spring (?? may be better:) boundary with stiffness k_1, that takes care of perfect-plastic repulsion, and a linear dashpot that accounts for dissipation during contact [8,9,12]. Elasticity at the contact level is added by a spring, with a larger stiffness k_2, for unloading and reloading, so that the stiffness increases due to irreversible deformations. Cohesion (or an adhesion force) between the contacts comes into the model by a "cohesive stiffness" k_c, which allows for attractive forces (here negative) up to a maximal attractive force f_{min}. The tangential force involves dissipation due to Coulomb friction, but also some tangential elasticity that allows for stick-slip behavior on the contact level [1,2,6,8].
If all forces acting on a selected particle (either from other particles, from boundaries or from external forces) are known, the problem is reduced to the integration of Newton's equations of motion for the translational and rotational degrees of freedom.

Simulation Results

The system examined in the following contains N=1950 particles with radii randomly drawn from a homogeneous distribution with minimum 0.5 mm and maximum 1.5 mm. The total mass of the particles in the system is about 0.02 kg. If not explicitly mentioned, the material stiffness parameters are $k_2=10^5$ N/m, $k_1/k_2=1/2$, and the contact-viscosity is 0.1 kg/s. The eigenfrequency of the particle contact is hence typically 10^{-5} s so that an integration time-step of 2.10^{-7} s is used, in order to allow for a "safe" integration [1,12].
Initially, the particles are randomly distributed in a huge box, with rather low overall density. Then the box is compressed, either by moving the walls to their desired position, or by defining an external pressure p, in order to achieve an isotropic initial condition. Starting from this relaxed, isotropic initial configuration, the strain ε_{zz} is applied to the top wall and the response of the system is examined. In Fig. 3, the volume change of simulations with different cohesion strength shows first compression and then dilatancy. The stronger the cohesion, the more the material can be compressed, while the dilatancy is almost un-affected by cohesion. At the same time, the stress response (index zz denotes the vertical stress) becomes more and more an-isotropic, i.e., the vertical stress increases until it reaches a maximum, while the horizontal stress remains constant. After the peak, softening behavior and large fluctuations are evidenced. The peak stress value increases with the microscopic cohesion or adhesion force f_{min}. A representative snapshot from this simulation is shown in Fig. 4.

The Macroscopic Material Behavior

From the macroscopic point of view, the flow behavior of the system can be examined by plotting Mohr-circles for different confining pressures (left-most point on the circle) and for the maximum stress (right-most point), see Fig. 5. The tangent to these circles can be seen as the flow function for the peak stress, which corresponds to a yield locus of an overconsolidated packing. It is linear for the examined parameters with a slope slightly larger than expected from the microscopic friction at the contacts alone. If no microscopic friction is active, a friction angle of about 13^o is obtained (0^o expected), while for a microscopic friction coefficient μ=0.5, the friction angle is about 30.5^o.(26.6^o expected).

When no adhesion forces are used or if the powder is practically free flowing, the macroscopic cohesion is non-existent, i.e., the flow function hits the origin, see Fig. 6. For increasing microscopic adhesion forces, the macroscopic cohesion also increases, following an analytical functional behavior as obtained from the microscopic contact model [8-10,12].

Summary

In the bi-axial box geometry, anisotropy in the stress response is observed during shear, but also strong inhomogeneities of forces and stresses, already in the initial isotropic situation can be evidenced. During deformation the stiffness and the anisotropy of the material increase until, going ahead with shear band localization, the material becomes softer and less an-isotropic. The critical state shear regime is not examined in detail here, see [11]. Increasing friction or cohesion leads to stronger material and, as a central result of this work, the macroscopic cohesion of the material is related to the maximal attractive adhesion force, see Fig. 5 (right).
Future work involves more detailed parameter studies and an extension of the method to three dimensional systems. The goal is then to quantitatively verify the simulations with experiments and eventually obtain constitutive laws from the model, based on microscopic parameters. This also involves a micro-macro transition procedure [6-8] for macroscopic fields like, e.g., deformation gradient, and stress, as developed recently.

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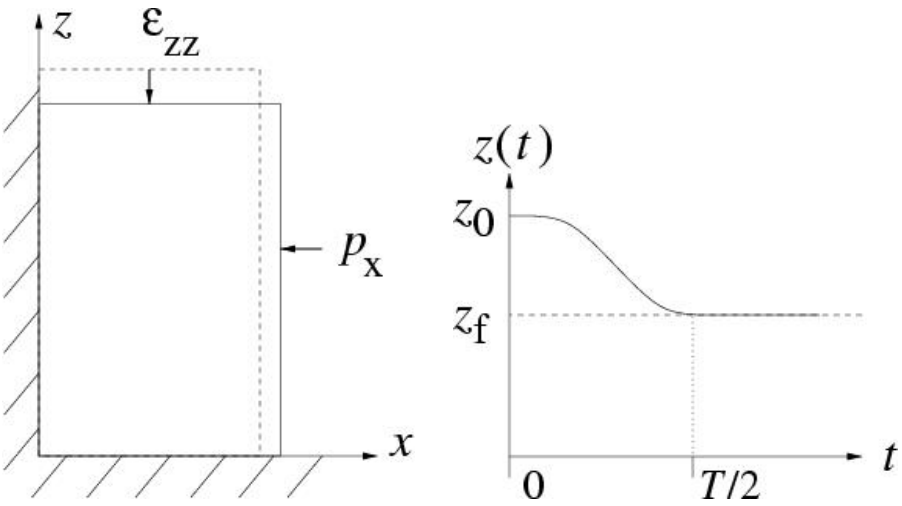

Figure 1 (left) Scheme of the model system; (right) top-wall motion as function of time

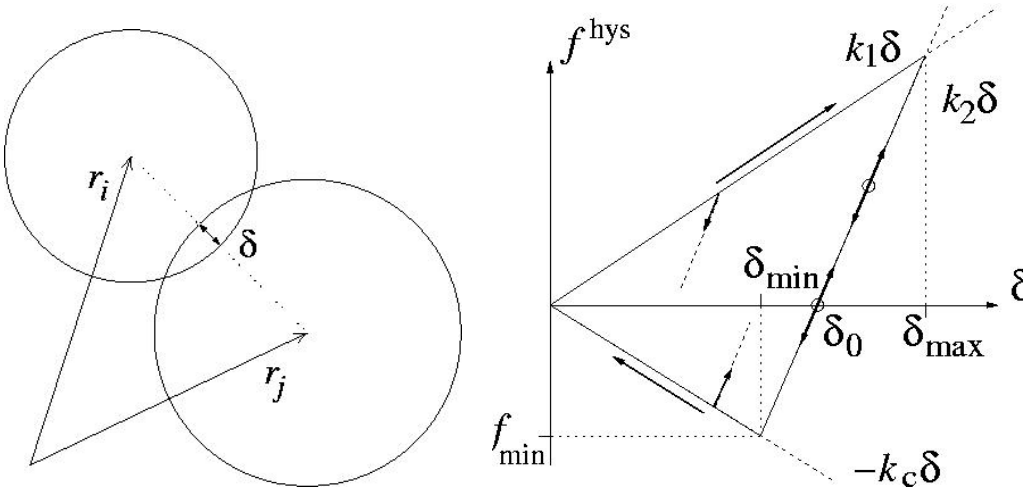

Figure 2 (Left) Two-particle contact; (right) force displacement law for the DEM simulations [12]

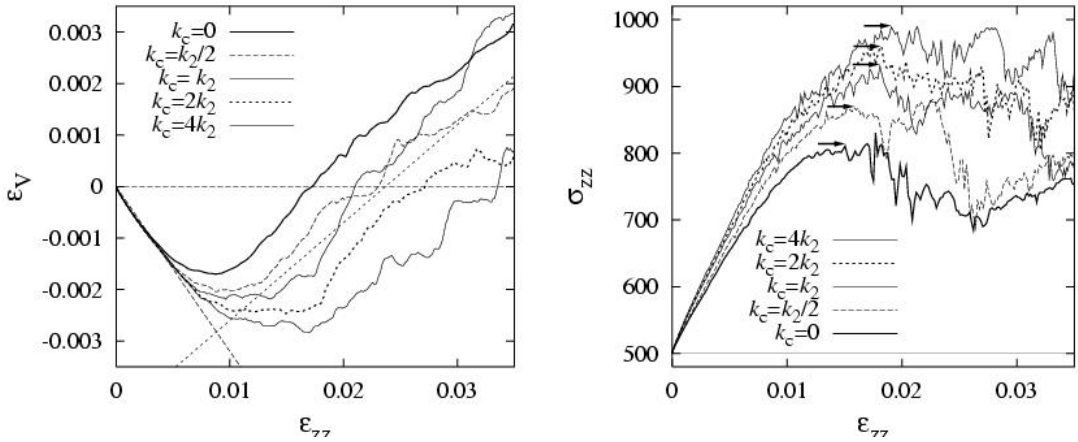

Figure 3 Volumetric strain (left) and stresses (right) during deformation

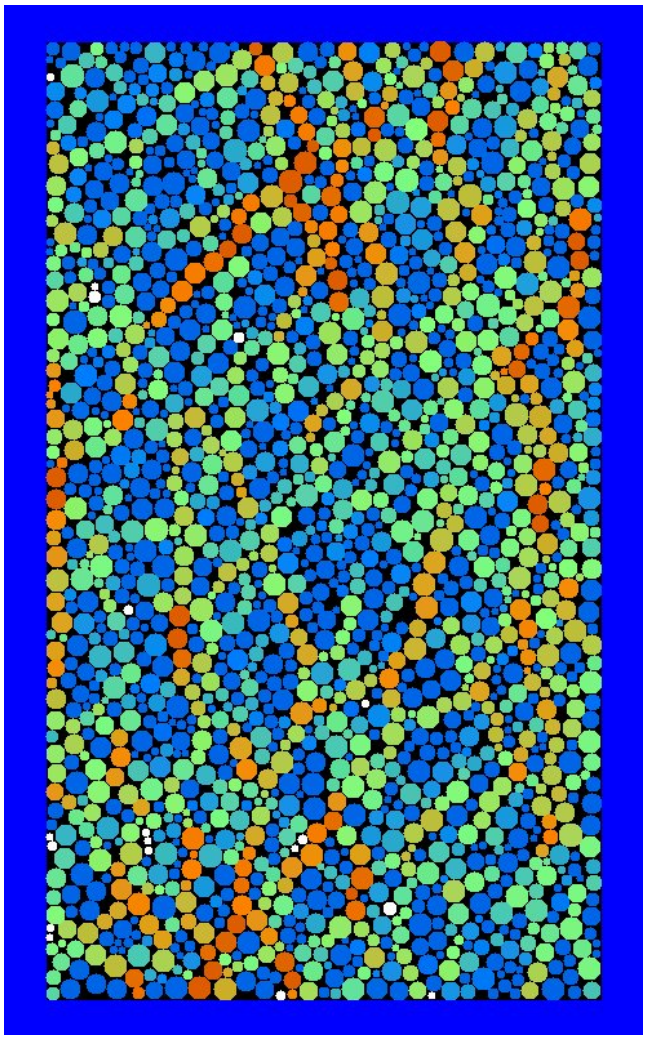

Figure 4 Snapshot from a biaxial box simulation with no cohesion at a strain of 0.042. Dark and bright particles correspond to small and large stresses, i.e., potential energy densities.

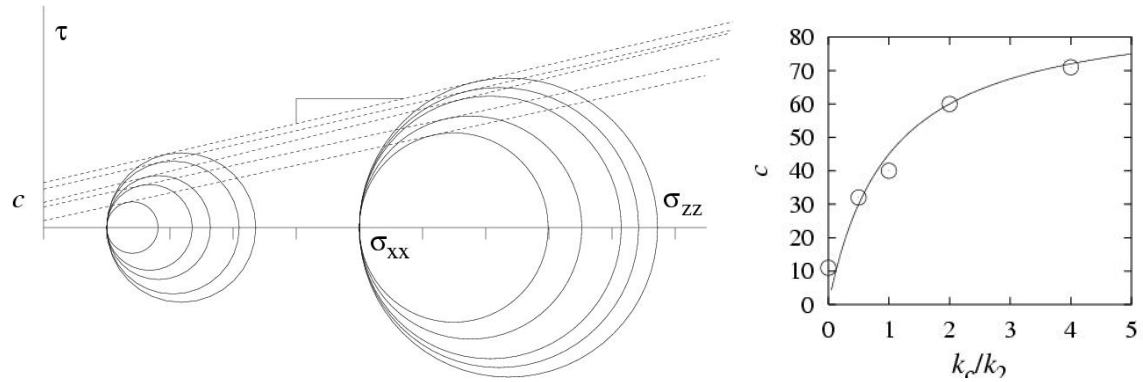

Figure 5 (Left) Mohr circle representation of the flow function at maximum stress for cohesion and no friction (Right) Macroscopic cohesion as function of the microscopic cohesive strength. The points are taken from the flow functions, the line corresponds to the analytical expression for the maximal attractive force as function of k_c/k_2

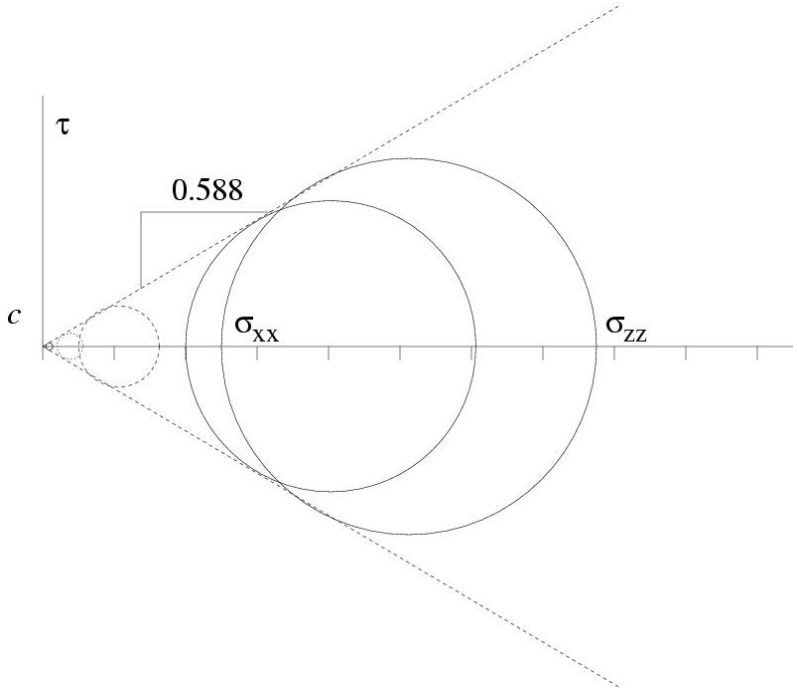

Figure 6
Mohr circle representation of the flow function at maximum stress for friction and no cohesion