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Micromechanical investigation of the fracture behavior of powder materials

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ABSTRACT

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Keywords: Powder compaction Fracture mechanisms Contact mechanics Experiments Discrete element method Green strength Fracture of compacted powder has been studied experimentally and numerically using a micromechanical approach. In the experimental investigation, the compacts are crushed in two different directions to account for general stress states and a microscopy study shows that fracture of the powder granules plays a significant role in the fracture process. The numerical analysis is based on the Discrete Element Method (DEM) and a novel approach is presented to account for the fracture of the particles in the numerical model. The force-displacement relations for two particles in contact, which are needed in DEM, are derived using micomechanical experiments together with finite element analyses of the contact problem. The contact model accounts for plastic compression, elastic unloading and adhesive bonding together with friction and tangential bonding. The model shows a very good agreement with the experimental data both for the elastic behavior during unloading and, if failure of the particles is accounted for, the fracture of the compacts.

shown in Fig. 1.

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1. Introduction

Compaction of powders followed by sintering is a popular production route of components of hard materials, like cutting tools, and components of complex shape. First, a die, shaped as the final product, is filled with powder material. The powder is pressed and the resulting compact, the green body, is ejected. The green body has very weak mechanical properties but from sintering the component gets its full strength but it also gets changes in its dimensions dependent on the density distribution. It is also of importance that the green body is crack-free before sintering due to the fact that green body cracks introduce weak zones and crack initiation points in the final products. In this context, it is obvious that modeling of the compaction process is of great importance for the product development.

The compaction process can, according to Ashby [1], be divided into three stages. The first stage, denoted stage 0, is the filling of the powder particles to a dense random packing. During the second stage, stage I, the particles indent each other at increasing compact density due to plastic deformations of the particles. The last stage, stage II, is characterized by the sealing off of the pores between the particles giving a mechanical behavior that is close to that of a porous solid.

In recent years micromechanical models of the powder compaction processes, and especially stage I compaction, have gained a lot of interest as these models rely on a physical description of the powder

* Corresponding author. *E-mail addresses:* erolsson@kth.se (E. Olsson), pelle@hallf.kth.se (P.-L. Larsson). [10]. If neither the elastic nor the plastic deformation of the contacting particles can be neglected, a semi-analytical treatment is possible in order to derive the contact forces, cf. [11] where the analysis is based on the correlation of hardness tests, originally presented in [12,13]. This correlation together with spherical contacts were studied in detail

particles instead of the more involved and more phenomenological models needed to describe the powder as a continuum. Pioneering

work in the field of micromechanical models were performed by

Wilkinsson and Ashby [2] followed by studies by Fleck et al. [3] and Fleck [4]. In all micromechanical models of powder compaction, the

most important part is the modeling of the contact behavior between

two powder particles and especially the normal contact force, F_N , as

function of the indentation depth, h. A sketch of the two particle prob-

lems together with a representative force-indentation relationship is

contact theory [5]. However, elastic contact models will only be appro-

priate during the filling stage as during the compaction, the particles un-

dergo large plastic deformations. Furthermore, for particles made of

materials with negligible elastic deformation and assuming power-law

hardening plasticity or creep, the contact problem is self-similar, when

relying on small deformation theory, as recognized by [6–8]. Under

such conditions, closed form solutions for the contact force exist. The

solution was then successfully used in analytical models of powder

compaction based on the assumption of affine motion of the powder

particles by [9] and in a more comprehensive study by Storåkers et al.

For elastic spherical particles, the function $F_N(h)$ is given by the Hertz









Fig. 1. Sketch of a representative force-displacement relationship pertinent to simulation of powder compaction.

by Mesarovic and Fleck [14,15] where it also was shown that large deformations heavily affect the contact problem and thus the validity of the analytical solutions is significantly reduced. Further progress to better correlate spherical indentation tests and more accurately describe the contact between spherical elastic–plastic bodies was made by Olsson and Larsson [16] and Larsson and Olsson [17].

To analyze unloading and the fracture strength of powder compacts using micromechanical models, which is the aim presently, models are needed for the unloading of the contact also accounting for the adhesive bonding between the particles. Regarding elastic particles, the solution has been known since the mid-seventies by the analysis from the JKR model, [18] and the DMT model, [19]. For contacts involving ideally plastic materials, Mesarovic and Johnson [20] provided the solution which was later extended to power-law hardening plasticity in [11].

As mentioned earlier, it is possible to derive analytical micromechanical models of powder compaction under the assumption of affine motion of the particles. Such models do not, however, take particle rearrangement into account and thus reduce the validity of the model especially in the case of uniaxial compaction. To overcome this short-coming, the Discrete Element Method (DEM) can be used which was originally developed by Cundall and Strack [21]. Early investigations of compaction using DEM include a plane strain study by Redanz and Fleck [22] and a full 3D study by Heylinger and McMeeking [23]. Using DEM together with the contact model from Storåkers et al. [8], Martin et al. [24], Martin and Bouvard [25], Skrinjar and Larsson [26,27], Olsson and Larsson [28] successfully analyzed isostatic and uniaxial cold compaction of equal particles and particles of different materials and size.

Regarding the present investigation, unloading and fracture of powder compacts, two studies were presented by Martin [29,30] where the previously mentioned contact model in [20] were used to describe the bonding between the powder particles. In all the above mentioned DEM studies, it is assumed that the mechanical properties of the powder particles are known. However, for many industrially relevant applications, for instance, spray dried powder granules which is the material studied experimentally here, the mechanical behavior is unknown. One solution, including both compaction, unloading and fracture, was presented by Pizette et al. [31] where the form of the force–displacement relationships were specified a-priori and a Design of Experiment (DoE) setup was used to determine the unknown parameters. The drawback with that method is that the force–displacement relations needs to be specified a-priori which could be difficult as demonstrated by the fracture strength simulations in [31] where the model only was able to fit the data at one particular compact density.

One feature that, according to authors' knowledge, has not been included in DEM simulations, and could be important in determining the fracture strength of powder compacts, is fracture of the particles themselves. There exist studies in the literature where the granules themselves are modeled using several thousand particles, cf. eg. [32,33] but when accurately simulating more than a few tens of granules the computational time becomes to long.

In short then, the aim with the present work is to analyze unloading and fracture of powder compacts incorporating both contact and particle fracture. The simulations will be carefully evaluated using two types of crushing experiments in order to scrutinize the effect of different parameters. This will be achieved by accomplishing the following tasks also defining the outline of the paper.

- An experimental study of the compaction, unloading and fracture of the powder compacts including a microscopy study of the fractured compacts in order to identify the fracture mechanisms. This study is presented in Section 2.
- A mechanical model describing the granule material based on micromechanical experiments. The requested model was presented in [34] but will be summarized in Section 3 for clarity.
- A mathematical model of the contact force between two contacting particles including all important effects needed to describe the forces acting on a particle based on the experiments in Section 2. This includes plastic deformation at compression, elastic unloading and bonding of the contact as well as friction. The mathematical model (in Section 4) is supported by single particle finite element simulations.
- A novel method for describing fracture of the individual particles is presented in Section 5 including both a fracture criterion as well as the post fracture behavior based on experimental observations.
- The discrete element method code, with all the incorporated features, is presented in Section 6.
- All experimental steps described in Section 2 is analyzed with the DEM program in Section 7 to critically evaluate the proposed model for the powder material.

2. Experiments

The experimental part of the work was performed using testing equipment from PTC [35]. The powder materials used in the experiments are two types of spray dried cemented carbide powders used in the industry with slightly different properties. The different powder materials are denoted Powder A and Powder B respectively. Both powder granules consist of small cemented carbide particles. The size of these particles is approximately 0.6 m for Powder A while the corresponding size in the case of Powder B is 3.6 m. The amount of binder, which is of the same type for both powders, polyethyleneglycol, is 2 wt.% for Powder A and 2.1 wt.% for Powder B. The granule size is approximately 100 m for both materials.

The density of the final sintered component, denoted D_{th} and reported in Table 1, will be used as a reference density for the calculation of the relative density D which is defined as the density of the compact divided by D_{th} . Also reported in Table 1 is the estimated inter-particle friction coefficient as well as the density after filling, D_{bulk} , and the density after shaking, D_{tap} , determined in [34]. The relative density of a single granule, D_{part} , which is needed in order to compare results from DEM simulations and the experiments, was computed using DEM in [34].

 Table 1

 Properties of the two investigated powders.

Powder	$D_{th}[g/cm^3]$	$D_{bulk}[g/cm^3]$	$D_{tap}[g/cm^3]$	$\theta_{rep}[^{\circ}]$	μ_{part}	D _{part}
Powder A	14.45	3.554	3.8	30	0.58	0.48
Powder B	14.64	3.382	3.571	32	0.62	0.46

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