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Plastically-driven variation of elastic stiffness in green bodies during powder compaction. Part II: Micromechanical modelling

L.P. Argani [a], D. Misseroni [a], A. Piccolroaz [a], D. Capuani [b], D. Bigoni [a,*]

[a] DICAM, University of Trento, via Mesiano 77, I-38123 Trento, Italy
[b] Department of Architecture, University of Ferrara, Via Quartieri 8, 44100 Ferrara, Italy

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ABSTRACT

A micromechanical approach is set-up to analyse the increase in elastic stiffness related to development of plastic deformation (the elastoplastic coupling concept) occurring during the compaction of a ceramic powder. Numerical simulations on cubic (square for 2D) and hexagonal packings of elastoplastic cylinders and spheres validate both the variation of the elastic modulus with the forming pressure and the linear dependence of it on the relative density as experimentally found in Part I of this study, while the dependence of the Poisson's ratio on the green's density is only qualitatively explained.

1. Introduction

Densification of metal as well as ceramic powders is a problem connected with a strong industrial interest, so that the micromechanics of this process has been the focus of a number of investigations (almost all addressed to metal particles, while the akin problem of ceramic powders has been much less investigated). Grains have been usually assumed as spherical (or cylindrical for simplicity), so that micromechanics explains how plasticity and increase of contact areas between particles influence the overall stress/strain behaviour. The analysis of this problem sheds light on the macroscopic constitutive modelling of the powder, to be employed in the design of moulds to form green pieces with desired shape. The compaction problem is also of great academic interest in several fields, including biomechanics, where it traces back to the famous 'Histoire Naturelle' by the Count de Buffon, who reports on a (probably 'thought') experiment with peas:

> Qu'on remplisse un vaisseau de pois, ou plutôt de quelqu'autre graine cylindrique, et qu'on le ferme exactement après y avoir versé autant d'eau [...]; qu'on fasse boullir cette eau, tous ces cylindres deviendront des colonnes à six pans. On en voit clairement la raison, qui est puramente mécanique; chaque graine, dont la figure est cylindrique, tend par son reflement à occuper le plus d'espace possible dans un espace donné, elles deviennent donc toutes nécessairement hexagones par la compression réciproque.

This is an example of compaction of a package of spheres (Fig. 1), later continued by D'Arcy Thompson in his *On Growth and Form* and others.

Micromechanical models of powder compaction have been developed so far for a cubic (square in 2D) geometry of spheres [1–4] or cylinders [5–8] in frictionless contact, and friction between grains has also been considered for the latter geometry [5]. Random packing of cylinders and spheres have been analyzed respectively in [4,5]. All the above-mentioned investigations, in which the spheres and the cylinders are modelled within the framework of the J_2-flow theory of plasticity with linear hardening or perfectly plastic behaviour (Fig. 6), are all focused on the determination of the yield surface at different stages of compaction.

The objective of the present article is to investigate how the *plastic deformation of grains* during compaction influences the macroscopic *elastic* response of the material, an aspect never considered before, but central in the development of elastoplastic coupling (see Part I of this study). To this purpose, 2D (plane strain) and 3D square/cubic and hexagonal packings of cylindrical and spherical grains are considered (Fig. 3). Although detailed information on the constitutive law valid for the grains is not available, these are modelled via von Mises perfect or linear hardening plasticity, which is typical of a basic and simple mechanical behaviour. Representative volume elements of the cylinder and sphere packings are deformed to model the state of uniaxial strain achieved in a cylindrical rigid die and the mean stress/mean strain behaviour is numerically determined using the finite element program Abaqus

* Corresponding author.
E-mail address: bigoni@ing.unitn.it (D. Bigoni).

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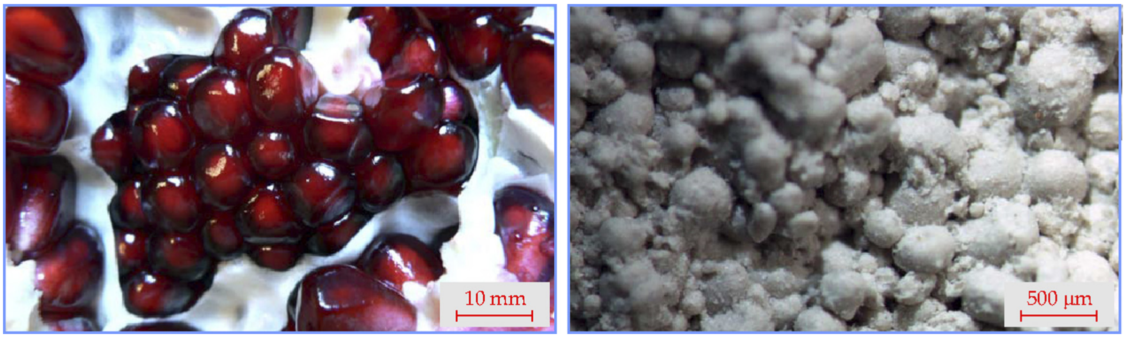
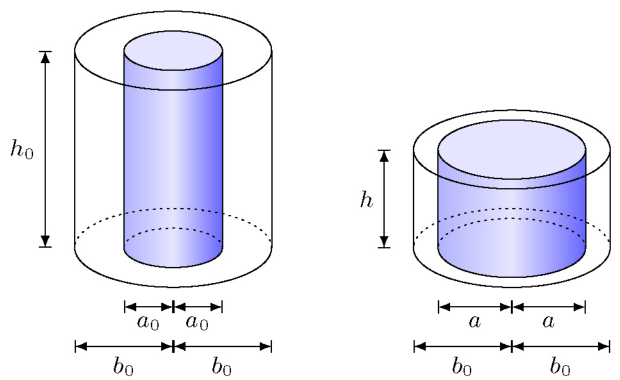


Fig. 1. Examples of packaged spherical particles in nature (pomegranate seeds, left, photo taken with a Panasonic DMC-FZ5 digital camera) and in industry (an aluminum silicate spray dried powder, right, photo kaken with a Nikon SMZ-800 optical microscope equipped with DSF1i camera head).



(a) *Unit cell undeformed configuration.* (b) *Unit cell deformed configuration.*

Fig. 2. A toy model to explain elastic stiffening due to plastic deformation. The elastic circular cylinder of initial radius a_0, height h_0, and elastic modulus E is coaxial to the unit cell of radius b_0. Upon axial plastic deformation, the inner cylinder has a radius a and height h ($a > a_0$ and $h < h_0$). If the plastic strain is isochoric $a^2 h = a_0^2 h_0$, so that the new geometry will result elastically stiffer than the initial one.

Unified FEA®. Once the uniaxial strain compaction has been completed, the representative element is unloaded and reloaded under uniaxial stress to evaluate the average Young modulus and Poisson's ratio of the material. In this way it is possible to determine the variation of the elastic modulus with the forming pressure and the dependence of the elastic modulus on the density. These evaluations validate the experimental results presented in the Part I of this study. The micromechanical evaluation of the Poisson's ratio is more complicated than that of the elastic modulus. In this case, the results from micromechanics correctly explain the qualitative increase of the Poisson's ratio with the forming pressure, but the values are not tight to experimental results.

The dependence of elastic stiffness on the level of plastic deformation is a crucial aspect of elastoplastic modelling of geological and granular materials, including ceramic, metal powders, and greens. Results provided in the present article explain the plastic micromechanisms inducing elastic stiffening during compaction of ceramic powders.

2. A toy mechanical model to explain elastoplastic coupling

Before to set up the micromechanical model for the qualitative and quantitative explanation of elastoplastic coupling, a simple mechanical model is presented with the aim of providing a simple explanation of the phenomenon. The model is intended only to shed light on the mechanism of increase in elastic stiffness due to plastic deformation and not to provide a quantitative evaluation.

Referring to an elastoplastic circular cylinder of initial height h_0 and cross section of radius a_0, this is inserted in a larger and coaxial cylindrical unit cell with cross section of radius $b_0 > a_0$ (Fig. 2), so that when the cylinder is subject to a force F (positive when tensile), the nominal stress is $\sigma_n = F/(\pi b_0^2)$, while the effective stress is $\sigma_e = F/(\pi a_0^2)$. Assuming that incompressible axial plastic deformation ε_p has brought the cylinder to a new height h and radius a, isochoricity implies $a^2 = h_0 a_0^2/h = a_0^2/(1+\varepsilon_p)$. The axial plastic deformation ε_p can be expressed in terms of void ratio as

$$\varepsilon_p = \frac{e - e_0}{1 + e_0}, \tag{1}$$

where $e_0 = (b_0^2 - a_0^2)/a_0^2$ is the initial void ratio and $e = (b_0^2 - a^2)/a^2$ is the current void ratio.

If the deformed cylinder is now loaded with a force F, the nominal stress remains equal to σ_n (because the radius of the unit cell does not change), but the deformation is $\varepsilon_c = F/(E\pi a^2)$, so that the apparent elastic modulus defined as $\bar{E} = \sigma_n/\varepsilon_c$ is

$$\bar{E}(\varepsilon_p) = E\frac{a^2}{b_0^2} = E\frac{a_0^2}{b_0^2(1+\varepsilon_p)}. \tag{2}$$

Eq. (2) is not expected to realistically represent the variation in elastic stiffness of a ceramic powder, but provides a simple model to understand the elastoplastic coupling effect at the microscale. In fact, for a compressive (and therefore negative) plastic deformation ε_p, the apparent elastic modulus of the material $\bar{E}$ increases, as it happens in a ceramic or metallic powder.

3. Micromechanical modelling

Square/cubic and hexagonal two-dimensional (grains are idealized as cylinders) and three-dimensional (grains are idealized as spheres) granule dispositions are considered as representative of ceramic powders, Fig. 3. Although at a first glance these geometries may appear far from the reality, they are usually considered to represent correctly the overall behaviour of granulates [1–8]. For the considered packagings, symmetry allows the reduction into the primitive cells and the unit cells shown in Fig. 3. For 2D (a quarter of a solid disk) and 3D (two eighths of a solid sphere) the reduction is shown in Figs. 4 and 5, respectively. The grains are in contact with smooth and rigid surfaces and all contacts between grains (and hence with the rigid surfaces) are assumed to be frictionless.

Reference is made to the ready-to-press commercial grade, 96% pure, alumina powder (392 Martoxid KMS-96), one of the three investigated in Part I of this study. This powder has particles of 170 μm mean diameter, obtained through spray-drying, and possesses a high plastic formability, because particles are made up of an aggregate of microcrystals with a polymeric binder. It is not known which constitutive equation models the material behaviour of the grains, except that it is an elastoplastic constitutive law. For this reason, the simplest constitutive framework of plasticity is