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Research paper

Numerical and experimental analysis of the Young's modulus of cold compacted powder materials

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ABSTRACT

We present co-designed experimental, theoretical, and numerical investigations aiming at estimating the value of the Young's modulus for cold compacted powder materials. The concept of image-based modeling is used to reconstruct the morphology of the powder structure with high fidelity. Analyses on aluminum powder pellets provide significant understanding of the microstructural mechanisms that preside the increase of the elastic properties with compaction. The role of the stress percolation path and its evolution during material densification is highlighted.

1. Introduction

Materials or components made from powders have enormous societal and industrial impact. To list some everyday examples: i) pharmaceutical tablets (Michrafy et al., 2002; Kadiri et al., 2005; Wu et al., 2005; Klinzing et al., 2010) are the most widespread use of compressed powder materials; ii) detergent tablets, a mix of surfactants, alkalis, bleaches, and other chemicals, are used in day-to-day chores; iii) candies are often created by compacting glucose powder with a small amount of binder. Structural and advanced materials also take advantage of compression technology. Cold compaction of ceramic powders (Piccolroaz et al., 2006a; 2006b) is extensively used in industry for advanced structural applications, such as chip carriers, and consumer products, such as tiles and porcelain. Powder metallurgy has a broad range of industrial applications, including manufacturing light engineering components and tools, along with bioengineering technologies (Laptev et al., 2016).

In many applications, the manufacturing process begins with cold compaction of powders (Fleck, 1995), performed using dies machined to close tolerances. This methodology enables powder cohesion through mechanical densification, which is governed by different mechanisms, including particle rearrangement, elastic and plastic deformations. The purpose of compaction is to obtain a *green* compact, with sufficient strength to withstand further handling operations, such as sintering.

Processing options permit selective placement of phases or pores to achieve targeted effective properties after cold compaction. The mechanical properties of green compacts are strongly influenced by the morphological characteristics of the compound. Micrographs of the particle arrangement show that the morphology of the powder pack changes with the forming pressure from an assembly with ideal point-wise contact to a severely plastically deformed state, with a substantial reduction of voids. This and other studies show that the Young's modulus varies with the stiffness of each phase and with the network of inter-particle contacts.

Tracking the contact regions between the particles while they experience large deformations is a formidably complex task (Gonzalez and Cuitiño, 2016) and is not the goal of this manuscript. This paper aims to estimate the Young's modulus of cold compacted metal powders via computational simulations using *image-based morphological reconstructions* of the microstructure and *high performance computing*. The work has sound motivations: whereas experimental investigations on the topic are covered by relatively broad literature, only a few numerical analyses have been carried out.

Experimental investigations on the elastic properties of cold compacted powders have been published by several authors, see Carnavas and Page (1998) and Argani et al. (2016b) and references therein, studying the effects of the powder morphology. Two major

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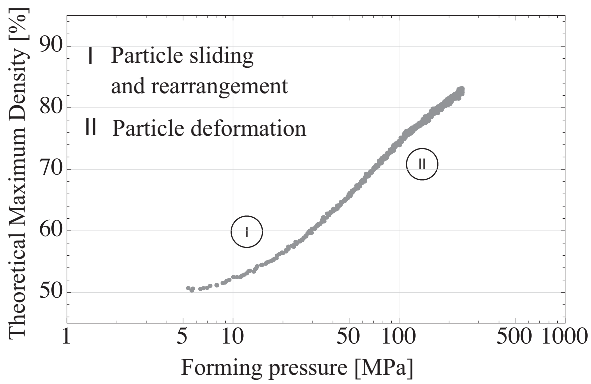


Fig. 1. An illustration of aluminum particle rearrangement, deformation, and densification during compaction. A sharp differentiation between these phases could not be precisely identified. Dots correspond to experimental data, which refer to the same powder compound used for Young's modulus estimation.

conclusions have been confirmed by the present numerical analyses, namely: i) the load response of lightly compressed powders is dominated by its particulate nature and inter-particle forces; ii) the load response of heavily compressed materials is similar to that of a porous solid. Our simulations provide further insight into the microstructural mechanisms that control the increase of the Young's modulus with forming pressure by highlighting the relevance of the stress percolation path generated by the contact areas between particles. Similar studies have been made by Kruyt (2016) and Kruyt and Antony (2007), as well as by Poquillon et al. (2002a; 2002b). The role of the rate of compaction was investigated more recently in Wang et al. (2009).

Literature on macroscopic models of metal powder densification under cold compaction is very broad (cf. Gu et al., 2001 and the references in Piccolroaz et al. (2006a)). Microscopic investigations have been carried out by studying the contact force distribution in idealized rigid (Kanatani, 1981) or deformable (Jefferson et al., 2002; Argani et al., 2016a) particles. Numerical analyses have been performed by the discrete (Makse et al., 2000) or finite (Argani et al., 2016a; Kim and Cho, 2001; Lee and Kim, 2002) element methods. By treating the powder material as a two-phase composite, effective properties can be extracted from the extensive literature on the subject - see for instance Torquato (2002). Numerical investigations in the present paper have been compared to the Hashin–Shtrickman bounds (Hashin and Shtrikman, 1962) and the boolean model of spheres (Serra, 1980; Stoyan and Mecke, 2005) - also termed overlapping spheres theory (Torquato, 1997; 1998).

Computational simulations have the capability to test virtual materials, allowing for major cost savings, provided that scientific predictivity is achieved. The present work pinpoints the relevance of the image-based strategy in this regard. It confirms insightful conclusions drawn on experimental basis about the micromechanics of the cold compaction by highlighting the role of morphology and its evolution during the forming process. Specifically, it brings attention to the fact that a unique value for the Young's modulus, especially at low volume fractions, may not be identified since it is severely influenced by the history of deformation and the generation of the stress percolation path (Radjai et al., 1998).

The paper is organized as follows. Section 2 comprises the Young's modulus measurements, as well as the full description of the powder compound and of the experimental setup. The notion of *image-based modeling* is discussed in the subsequent section, highlighting the fundamental tasks of data acquisition, the construction of percolation paths, and the statistical and the numerical analyses. Results are discussed in Section 4, assessing numerically several insights provided on experimental basis.

2. Experimental evidence

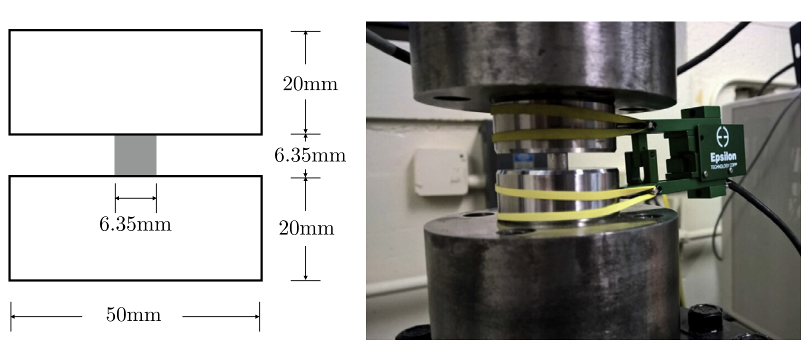
Powders (99.8% pure Al with -100+325 and -325 mesh size) have been purchased from Alfa Aesar. They have been sieved for 24 h using a sieve shaker (RO-TAP RX-29) to a particle size range of 106–355 µm. Young's modulus has been measured from the sieved as-received and high-energy ball milled Al powders. The milling procedure and results for high-energy ball milled Al powders are reported in Appendix A.

2.1. Quasi-static measurement of Young's modulus

Pellets ranging from 80 to 98% theoretical maximum density (TMD) were cold pressed from the sieved Al powders in a 6.35 mm die purchased from MTI Corporation at a 1:1 aspect ratio. By increasing the amount of forming pressure, powder materials were transformed from a granular to a dense state in different phases, which have been plotted in Fig. 1.

The faces of the pellets were sanded to a flatness of approximately 10 µm. The samples were then loaded in 300 N/step increments in a uniaxial configuration, shown in Fig. 2. Graphite powder was used between the steel platens and the compact surface to reduce the effect of friction. The changes in the height of the pellets were measured using an Epsilon 3542 Axial Extensometer attached to the platens above and below the samples with the signal being recorded on a Tektronix 3054b oscilloscope. The relative density of the pellets was calculated after the experiment by measuring the pellet height, diameter, and mass.

The total measured displacement, δx_{tot}, is the sum of the displacement due to the measured portion of the plates, δx_{sys}, and of the sample, δx. Combining Hooke's law ($\sigma = E\varepsilon$) with the definition of engineering strain ($\varepsilon = \delta x / L$) and engineering stress ($\sigma = P/A$), the displacement due to the deformation of the sample is



(a) (b)

Fig. 2. Experimental setup for uniaxial compression experiments.