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The study of relations between loading history and yield surfaces in powder materials using discrete finite element simulations

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A B S T R A C T

Only a few studies in the literature have applied the finite-element method to analyse assemblies of meshed particles. These studies illustrated the relevance of this method for granular materials. Here, the compaction of ductile metal powders was studied through a numerical assembly of elastic–plastic and rate-independent spherical particles. The aim of this paper was to understand the evolution of yield surfaces with complex loading paths up to high relative density at the macroscopic scale and at the granular scale. Simulation results revealed that yield surfaces evolved with both isotropic and kinematic hardening mechanisms, depending on the compaction stage. An analysis of the sample microstructure was proposed, and a detailed study of contacts between particles revealed some of the mechanisms that led to the observed evolution of yield surfaces.

1. Introduction

Properly controlling the mechanical behaviour of ductile powders is a central issue in powder metallurgy. A key step of this process is cold compaction of powders, which allows the machining stages to be significantly reduced, and substantial cost savings. The aim of modelling is to predict the stresses on the tools and inside powder parts, to predict the density distributions, and to predict the mechanical strength of green parts. Another central issue is the prediction of the cracking phenomena, which are caused by deviatoric stress states that occur in small regions during the compaction stage. In this context, the evolution of stresses must be accurately reproduced to predict such singularities.

Both practitioners and researchers currently use numerical simulations coupled with continuum models for stress prediction. These models are often based on the Drucker-Prager Cap model (for instance, ABAQUS, 2009; Chtourou et al., 2002; Azami and Khoei, 2006), but they have several limits that have been underlined by experimental results (Akisanya et al., 1997; Pavier and Dorémus, 1999; Sridhar and Fleck, 2000; Schneider and Cocks, 2002). In particular, they cannot account for compaction-induced anisotropy.

However, technical problems related to experimental difficulties make the formulation of more adequate models complex. Triaxial experiments only give information on a limited number of loading paths. As a result, models do not correctly reproduce the response of powders to complex loadings, and no experimental results can be obtained.

Micromechanical modelling, an approach based on the modelling of individual particles, has been developed to circumvent these experimental difficulties. This approach allows the study of the links between the behaviours of the particle and the macroscopic material, through analytical or numerical methods. The approach requires simplifications on

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several levels, particularly on the geometry of particles and on the modelling of contacts. However, analytical models and numerical simulations:

- allow micromechanical phenomena such as friction and cohesion to be uncoupled from the global behaviour of the material;
- describe stresses, strains and displacements at the particle scale, which are not available using experimental devices;
- make the study of complex loading paths which are impossible to reproduce through experimental devices feasible.

For these reasons, the micromechanical approach is the only one that can aid in the understanding of granular phenomena and the consequences of these phenomena on the macroscopic behaviour of powders.

In the present work, micromechanical modelling was applied to probe the yield surfaces. The first micromechanical models that described yield surfaces were purely analytical (Fleck et al., 1992; Fleck, 1995; Storåkers et al., 1999). More recently, the Discrete Element Method (DEM) has been used to apply numerical simulation to the determination of the yield surfaces of granular media. The results were an improvement compared to former analytical models because the method considered rearrangement in a more natural way (Heyliger and McMeeking, 2001; Martin, 2004; Pizette et al., 2010).

However, analytical and DEM approaches are limited by theoretical modelling of contact stresses between discrete particles. The limits include the nonlinearity of the deformations and the complexity of the interactions between contacts around particles, which are approximated by contact models. Most of the previously cited results are based on the modelling of contact between elastic–plastic solids by Hill et al. (1989), Biwa and Storåkers (1995), Storåkers et al. (1997), but the application of this model to powder compaction is only valid for relative densities less than approximately 0.8–0.85 (Storåkers et al., 1999; Martin et al., 2003).

The extension of DEM to the field of high relative density is possible (Harthong et al., 2009). Although this approach has greatly increased the range of the relative density attainable with DEM, it has its own limitations. In particular, the contact surfaces and the particle deformation were not described in this approach; finite-element analyses of discrete particles assemblies had to be used to obtain this information with very good accuracy. With this method, referred to as Multi-Particle Finite-Element Method (MPFEM), particles are meshed, such that their deformation could be accurately described, unlike DEM in which rigid particles overlap each other. The first MPFEM studies (Gethin et al., 2001, 2003; Xin et al., 2003; Procopio and Zavaliangos, 2005) were limited to 2D configurations, because of the required calculation time. 3D simulations were conducted by Chen et al. (2008), Chen (2008) and Frenning (2008, 2010). Chen et al. (2006, 2008) and Chen (2008) also compared MPFEM numerical simulations using commercial finite-element software ABAQUS (2009) with experimental results on assemblies of millimetre-sized lead spheres. Their results showed the ability of MPFEM to correctly reproduce the behaviour of several assemblies of lead spheres.

Using MPFEM, Xin et al. (2003) obtained yield surfaces with periodic lattices of 2D particles, whereas Procopio and Zavaliangos (2005) obtained yield surfaces with randomly arranged 2D particles, and Schmidt et al. (2008) obtained 3D yield surfaces obtained from a random assembly of 50 spheres. The MPFEM has the advantage of taking all granular phenomena into account. It is also able to consider irregular particles within the limits of mesh refinement (Gethin et al., 2006). Moreover, MPFEM only requires the modelling of the constitutive material of the particles and the interfacial behaviour, that is, friction and if necessary, cohesion.

The present paper reports the characterisation results of granular materials, with the formulation of a continuum constitutive law for the compaction of ductile powders as the ultimate goal. The paper presents simulation results (which may be considered as numerical experiments) aimed at characterising the evolution of yield surfaces with the loading path, and a micromechanical interpretation of these results. Section 2 describes how the method was implemented. Section 3 presents the yield surfaces obtained from modelling with various loading paths. A micromechanical analysis focused on the understanding of the phenomena that cause the observed evolution of the yield surfaces is proposed in Section 4.

2. Method

2.1. Principle of the method and the probing of yield surfaces

First, the method required a numerical sample, or an assembly of spheres, to be defined as a powder sample. The details of defining this assembly will be given in Section 2.2. This sample was then modelled in the commercial finite-element code ABAQUS. Simulations were then performed to apply different loading paths and to study the mechanical response.

In the present study, the constitutive material was the same for all particles in the assembly. It was modelled as an elastic–plastic material with isotropic and linear elasticity. The elastic modulus was defined as E and the Poisson coefficient was defined as ν. Since the typical size of real powder particles usually range between 10 and 100 μm, it was assumed that the plastic behaviour of the constitutive material of the particles could be modelled using Von Mises criterion and the model included strain hardening. Details of the model implementation can be found in ABAQUS user documentation (ABAQUS, 2009). Strain hardening was defined by the following relation:

$$\sigma = K\varepsilon^n \tag{1}$$