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Micro Mechanical Modelling of Compaction of Metallic Powders

F.Kalantary[1] and G.N.Pande[2]
Guilan University,
Rasht, Iran.

Abstract

The micro mechanical behaviour of ordered packing of powders with spherical grains under isostatic compaction was studied using an "Updated Lagrangian", large strain, elasto-plastic finite element program, developed for this purpose. An appropriate contact algorithm was developed in conjunction with this program to handle the discrete nature of the problem. Cubic and hexagonal rhombohedral packing were considered. A repetitive cellular unit pattern was deduced and the numerical simulation of its compaction process was carried out.

The effect of different material properties on the variation of compaction pressure with specific volume (density) was examined. The effect of elevated temperature in the Hot Isostatic Pressing (HIP) on the compaction process was also considered.

Keywords: Powder – Compaction – Micro Mechanical – Finite Element

Introduction

With ever-expanding application and demand for the powder technology products, it has become apparent that an accurate mathematical model of the compaction process is of paramount importance. Compaction constitutes an important part of the production route, which not only affects the mechanical properties of the produced article, but also ranks high in economic and design considerations. Therefore, a mathematical model that facilitates reliable prediction of the powder response under various compaction forces is highly desirable. However, a comprehensive rationalization of the mechanics of particulate materials has so far evaded the engineers for a variety of intricate reasons. The discrete nature of granular materials, as well as the random manner in which particles interact are the most notable causes for this lack of total success. A great number of attempts have, nevertheless, been made to elucidate the problem from a variety of viewpoints. In this respect, micro mechanical study of discontinuous media has gained widespread recognition in recent decades. It is often argued that a thorough description of the behavioural pattern of particulate materials is impossible without due attention to the discrete phenomenon that occurs at particle level. [1]

This has generated an upsurge in micro mechanical study of granular substances. Various techniques and approaches have been attempted in order to quantify the micro mechanical behaviour of powder masses and to draw conclusions as to its effect onto the macro-scale response of the medium. For instance, extensive work has been undertaken to explain the anisotropy of some granular materials through micro mechanical concepts [1,2,3]. Also numerous attempts at modelling cold or hot compaction and sintering processes have been concerned with the study of unit cell models [4,5,6,7].

Meanwhile, other researchers have pursued the line of depiction of granular materials response in terms of evolution of topological features of the materials, [8,9] or qualitative simulation processes, [10,11] or derivation of probabilistic and statistical parameters [12,3] for the description of particle interaction under loading.

[1]Assistant Professor, Faculty of Engineering,
Guilan University, Iran
[2] Professor, Faculty of Engineering,
University College, Swansea, Wales, UK

By and large, although these attempts have not been completely successful in predicting the macro-mechanical behaviour, but have nevertheless helped a great deal in clarifying various intricate micro mechanical characteristics. It is therefore proposed here to pursue the line of unit cell models using numerical simulation techniques.

Unit Cell Model

Many of the metallic powder production techniques, produce virtually mono-size, spherical particles which when poured into a die would pack in either cubic (rhombohedral or orthorhombic) or hexagonal (rhombohedral or tetragonal) arrangements (figure 1)[13]. Since rhombohedral cubic and hexagonal packing are probabilistically the most viable of the natural arrangements of powders, it is proposed to base the micro mechanical model on these two regular packing orders.

Due to the deterministic nature of the packing, a repetitive cellular pattern emerges and thus the problem reduces to simulation of compaction of symmetrical unit cells, depicted in figure 2. This approach is the inverse of Gadala's[4] attempt to provide a finite element solution to Green's model, where the material is assumed to contain a regular array of cubic and hexagonal voids. The approach has also been independently suggested by O'Donnell and Steif [14]. Some similar results have also been presented by Williamson et al [15].

Numerical Solution

Since powder compaction involves large plastic deformations of the grains (Figures 3a and 3b), the process is simulated by an elasto-plastic, large strain, "Updated Lagrangian" finite element program in conjunction with a linear contact algorithm [16].

The Updated Lagrangian formulation is based on the same procedure as for the Total Lagrangian formulation, except that the equilibrium equations are written with respect to an updated equilibrium configuration and not the initial state and all static and kinematic variables are also measured with respect to this same configuration. This configuration may be any already defined state, but usually it is the most recent equilibrium state [17].

The equation of motion for Updated Lagrangian formulation must therefore be stated as:

$$R^{t+\Delta t} = \int_{V^t} S_{ij}^{t+\Delta t}\,\delta E_{ij}^{t+\Delta t}\,dV^t \qquad (1)$$

Where S_{ij} is the second Piola-Kirchhoff stress at time $t+\Delta t$;

$$S_{ij}^{t+\Delta t} = S_{ij}^t + dS_{ij} \qquad (2)$$

and since at time t the second Piola-Kirchhoff stresses are identical to Cauchy stresses σ_{ij} [18]

$$S_{ij}^{t+\Delta t} = \sigma_{ij}^t + dS_{ij} \qquad (3)$$

The Lagrangian strain tensor used in Updated Lagrangian formulation is often taken [17] to be;

$$dE_{ij} = \frac{1}{2}\left[\frac{\partial(du_i)}{\partial x_j} + \frac{\partial(du_j)}{\partial x_i} + \frac{\partial(du_k)}{\partial x_j} \bullet \frac{\partial(du_K)}{\partial x_i}\right] \qquad (4)$$

Where the differentiations are performed with respect to the current coordinates X_i.

In a similar fashion to the Total Lagrangian formulation the Lagrangian strain increment dE_{ij} may be decomposed into a linear and a nonlinear part;

$$dE_{ij} = d\varepsilon_{ij} + d\eta_{ij} \qquad (5)$$

Where;

$$d\varepsilon_{ij} = \frac{1}{2}\left[\frac{\partial(du_i)}{\partial x_j} + \frac{\partial(du_j)}{\partial x_i}\right]$$

$$d\eta_{ij} = \frac{1}{2}\left[\frac{\partial(du_k)}{\partial x_j} \bullet \frac{\partial(du_k)}{\partial x_i}\right]$$

Hence the equation of motion may be stated as;

$$R^{t+\Delta t} = \int_{V^t}\left(\sigma_{ij}^t + dS_{ij}^t\right)\ \delta\left(dE_{ij}\right)dV^t \qquad (6)$$

Since $\delta\left(E_{ij}^t + dE_{ij}\right) = \delta\left(dE_{ij}\right)$.

Hence the final incremental equation of motion may be stated as; [17]

$$R^{t+\Delta t} - \int_{V^t} \sigma_{ij}^t\,\delta\left(d\varepsilon_{ij}\right)dV^t$$

$$= \int_{V^t} C_{ijkl}^{*}\,d\varepsilon_{ij}\,\delta\left(d\varepsilon_{ij}\right)dV^t + \int_{V^t} \sigma_{ij}^t\,\delta\left(d\eta_{ij}\right)dV^t \qquad (7)$$

Noting that $dS_{ij} = C_{ijkl}^{*}dE_{kl}$ and higher order terms have been omitted. Where again C^{*}_{ijkl} is usually an appropriately defined constitutive relation tensor for large strain formulation, but can also be taken as normal elasto-plastic constitutive relation.

The validity of the solution procedure, comprising of the large deformation solution algorithm and the contact detection algorithm was verified separately. The Updated Lagrangian algorithm was checked against the numerical test example of stretching of a perforated plate given by Zienkiewicz [19]. The contact detection algorithm was compared with the Hertz analytical solution and experimental data [20].

Material Properties

The basic material model chosen for the powder grain was linear elastic – ideal plastic. The elastic properties were E=100GPa and v=0.3 and the material non-linearity was modelled using a non-hardening Von-Mises yield criterion with associative flow rule and the yield strength was assumed to be σ_y=200MPa.

In order to study the effect of various parameters the following range of material properties were also examined against the basic parameters.

Modulus of Elasticity E= 100, 80, 60, 40, 20 GPa

Yield Strength σ_y= 300, 250, 200, 150, 100 MPa

Furthermore, in order to study the effect of various hardening parameters, the following hardening moduli for a hyperbolic hardening law were examined against an initial yield strength of σ_{yo}=100MPa and a ultimate yield strength of σ_{yu}=200MPa to match with the basic example:

H'=1, 2, 3, 4 GPa

Pressure-Specific Volume Plots

The variation of pressure with respect to specific volume is of utmost importance in cold compaction, since not only this determines the final mechanical and sintering characteristics of the work piece, but also it is the most relevant parameter in derivation of work hardening law.

Here, initially, the effect of elasticity modulus and yield strength on this relationship is examined. Figures 4a and 4b show the variation of isostatic compaction pressure verses specific volume for the range of elastic modulii for the two unit cells with a constant yield strength (σ_y=200MPa). It is evident from these plots that compaction pressure/specific volume relation is independent of the elasticity modulus. In other words it may be stated that the elastic rigidity has no bearing on the compaction process except for the very brittle grains which instead of plastically deforming, will crush and break down

Figures 5a and 5b present the variation of pressure/specific volume for a range of yield strengths with constant modulus of elasticity (E=100GPa). In contrast to the elastic modulus, yield strength has a significant effect on the pressure/specific volume variation and on the final pressure values. This is of course as expected since the shear strength is the characteristic that gives solid materials its resistance to flow.

Once again it may readily be noted that there is no difference in the pattern of progression of compaction curves between the two cell types, and the ultimate values of pressure are identical for various yield strengths of the two unit cells.

From the yield-normalized plots of these curves (Figures 6a and 6b), however, it may be seen that the pattern of compaction of all curves are identical, irrespective of the yield strength. It may also be noted that the ultimate pressure value for full compaction is approximately three times the yield strength irrespective of cell types, which confirms the reports in the journals [21,22].

This fact suggests that the initial specific volume has no influence on the ultimate value of compaction pressure necessary for full compaction, provided the material properties are the same.

Figures 7a and 7b present the effect of various hardening moduli on the compaction curves. It may be noted that in spite of the fact that variation of compaction force with specific volume is different for different hardening moduli, but the final compaction force necessary for full compaction is the same. This is explained by the fact that the ultimate value of yield strength is attained in all cases due to large plastic deformations different hardening moduli only affect the rate of this attainment and not the final value.

Temperature Effect

It is a well-known fact that in Hot Isostatic Pressing (HIP) as well as pressureless sintering processes, (compacted) powder particles exhibit viscous flow and diffusive transport due to the effects of high temperatures. This viscous flow and diffusions promote interparticle neck (contact) growth that constitutes an important aspect of densification process.

The viscous flow (or sometimes better known as creep) is a phenomenon well acquainted in engineering. However, when environment temperature is close to room temperature, creep can usually be detected if the material is subjected to sustained and prolonged loading, whereas in "*hipping*" and sintering processes, the elevated temperatures soften the material (i.e. increase ductility and reduce shear strength) to an extent that even the secondary force effects, such as capillary forces, surface tension forces and minute body forces can exercise a major influence on the flow mechanisms in a relatively short time span.

The hardness and strength of crystalline materials depend on dislocation mobility. Any phenomenon that hinders the motion of dislocations, increase hardness and strength but decreases ductility and

visa-versa. Mobility increases with temperature and physical properties change accordingly.
The numerical model used here for grain compaction is basically rate-independent and hence in the simulation process, the creep effect within the time frame cannot be accounted for. However, the effect of temperature is in a way exhibited through variation of yield strength. This is, of course, based upon the fact that shear strength of material is inversely proportional to the temperature and noting that the dependence of the yield strength on temperature varies for different materials. Therefore, provided that the variation of yield strength with temperature is known for the material, the pressure/specific volume variation may be scaled down accordingly.

Conclusion

Although the micro mechanical model of the compaction process proposed here is a simplified representation of the actual phenomena, it nevertheless has been shown to be capable of capturing some subtle characteristics of such a process. The collapse load was found to be about three times the yield strength, which ties in well with many previously suggested values [21,22].
A number of intricate details of the powder compaction have also been unraveled: From the pattern of propagation of plasticity region it appears that even at full compaction the central core of the grain remains unaffected by plasticity. This may have a direct bearing on any hardening postulates since hardening occurs where plastic flow has taken place. Hence at the end of compaction of a hardening material, the yield strengths of various regions of the grains are different.
The effect of temperature incorporated through variation of yield strength is shown to have a translatory role on the pressure/specific volume variation, rather than changing the whole process. Hence hot pressing may be simulated by simply evaluating the corresponding yield strength associated with that temperature.
Due to the fact that the present compaction model is only concerned with the latter part of the compaction process of powders (i.e. crushing of the grains) and consequently excludes any compaction due to re-arrangement of particles, a one to one comparison of this model with experimental data is not possible. In some cases a significant part of compaction occurs as a result of re-stacking and re-arrangement of particles, which is not modelled here. However, if this model were to be incorporated into a more global model that deals with the frictional deformation of the granular material, a better picture of the over all process would emerge.

Acknowledgment
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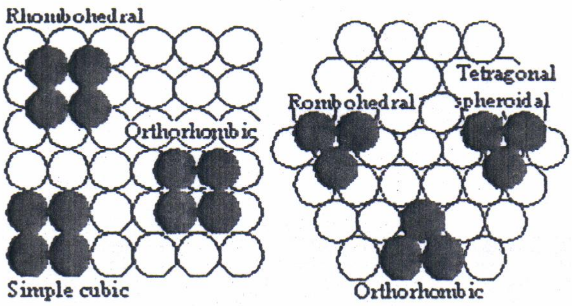

Fig.1. Packing orders.

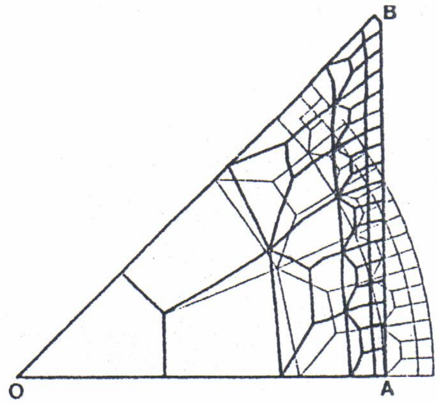

Fig.3a Cubic cell deformed mesh

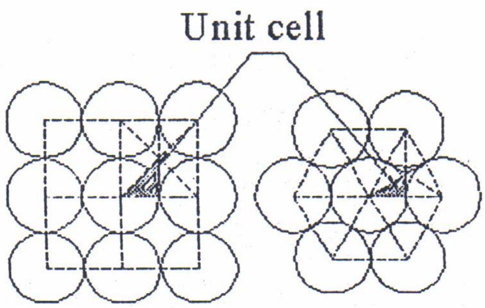

Fig.2. Unit cell presentation.

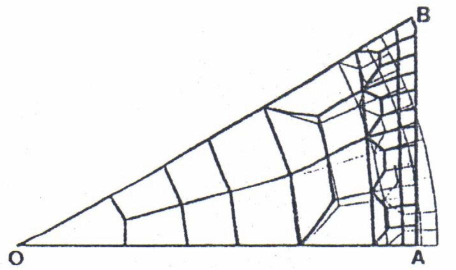

Fig.3b. Hexagonal cell deformed mesh

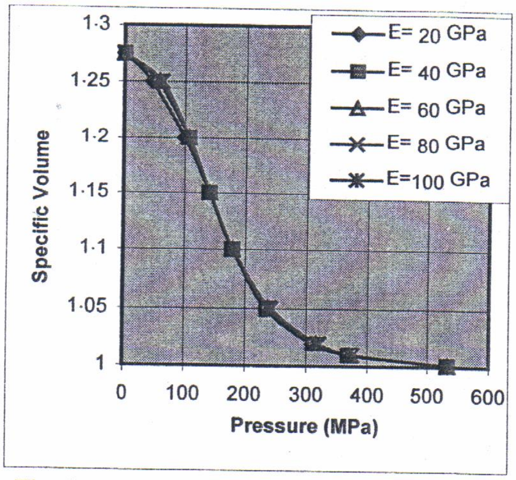

Fig. 4a. Effect of modulus of elasticity (Cubic)

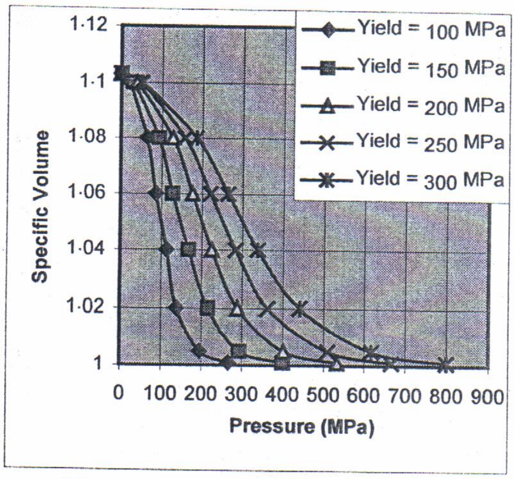

Fig.5b. Effect of yield strength (Hex.)

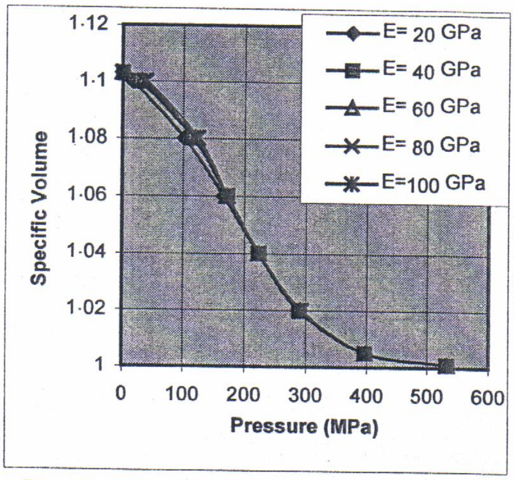

Fig. 4b. Effect of Modulus of elasticity (Hex.)

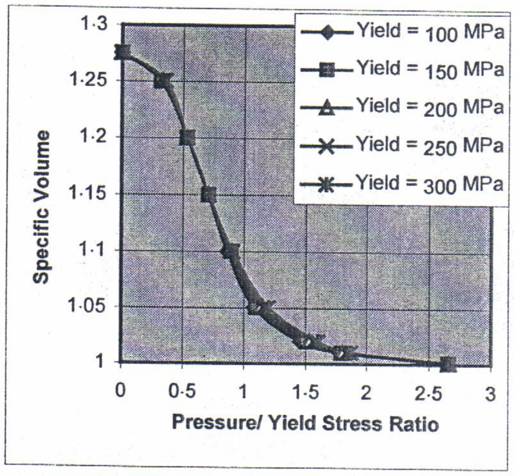

Fig.6a. Yield-normalized plot (Cubic)

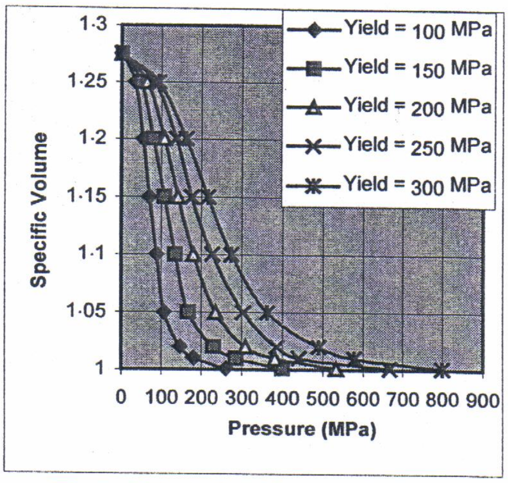

Fig.5a. Effect of yield strength (Cubic)

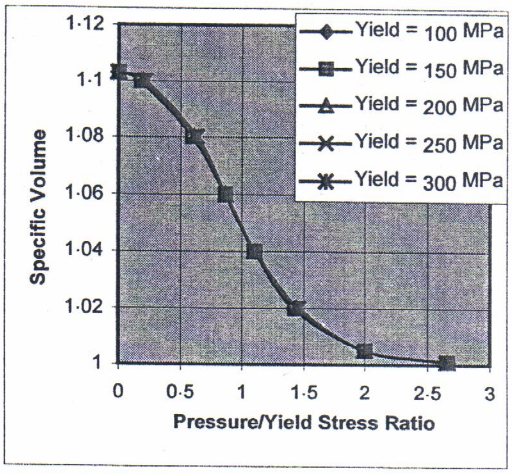

Fig.6b. Yield normalized plot (Hex.)

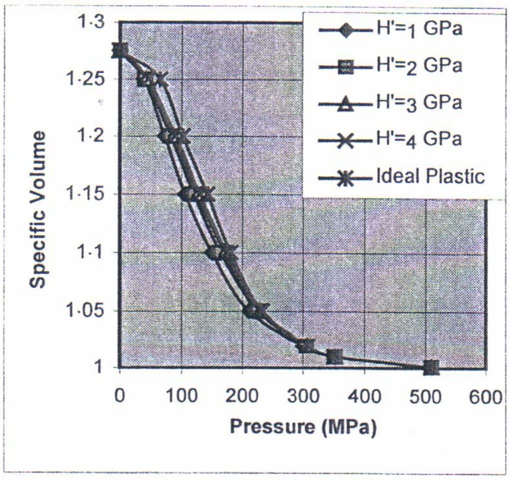

Fig.7a. Effect of hardening modulus (Cubic)

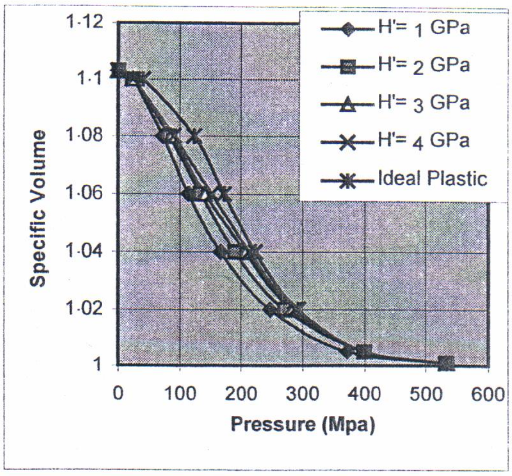

Fig.7b. Effect of hardening modulus (Hex.)