M. Powder Metal Performance Modeling of Automotive Components

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Objective

- Develop and evaluate math-based models for powder metallurgy component design and performance prediction. An existing U.S. Automotive Materials Partnership (USAMP) microstructure-property model for castings will be extended to powder metallurgy (P/M) for practical application in low strain-rate (design and durability) and high strain-rate (toughness-driven impact strength) environments. This model will be utilized to evaluate and optimize two component designs (a main bearing cap and a gear) as affected by material and manufacturing processes (compaction and sintering), and will accommodate each

companies' analytical codes (Abaqus, LS-Dyna, Ansys, etc.). The flexibility of this model will facilitate the evaluation of lightweight materials (such as aluminum and titanium) for future component applications.

Approach

- Determine current powder metallurgy standards publications, component design guidelines, manufacturing, and evaluation methodologies. Provide a selection of metal powders that can satisfy design performance requirements, component design guidelines, and manufacturing and testing specifications across industry participants (Task 1)
- Evaluate and develop numerical modeling techniques to predict mechanical properties throughout P/M component sections. The transition of current materials and designs to process structural automotive P/M components creates the need to predict the properties of the component in all sections of the design. In addition, there is the necessity to provide the least-cost, lowest-mass product designs and reduced development lead-time. Adapt and/or re-develop existing math-based models which are capable of accurately predicting P/M component structures and properties throughout the compaction and sintering processes (section size, density variation, dimensional tolerances, potential for cracking), alloys and process parameters (machine functions, tool and powder temperatures, strain rate, friction and pressure). Capture the history of a P/M part through its pressing, sintering, and life-cycle performance history using the developed multiscale methodology. (Task 2)
- Develop component and vehicle-level testing to validate durability, quality control and performance of P/M automotive parts. Quality control for P/M parts production involves several process factors such as powder properties, press settings, tooling design, and furnace condition. Determine these process factors in terms of their impact on process variations and quality improvement. Use optimization and statistical techniques to help determine the main factors affecting the final component. Perform validation experiments in which actual boundary conditions from real processes will be used to fracture the components. This will ensure us understanding the quality effects on the product along with the modeling effort. (Task 3)
- Manage and report program activities. The proper execution of this task will greatly enhance the value of the overall program. The type of reports and guidelines, which will be generated form this program will be in accordance with DOE and USCAR requirements. (Task 4)
- Perform Technology/Commercial transfer throughout the automotive value chain. Unlike aluminum, plastics and steel, there are no major R&D/technical institutions fostering the necessary infrastructure to support the large-scale application of automotive P/M components. It is for this reason, that if the auto industry wishes to take advantage of P/M's potential weight and cost reduction opportunities, it will have to nurture it through programs sponsored and directed by USCAR. The project team will request the professional support of societies to publish notices of meetings, and project information as released by the project team. (Task 5)

Accomplishments

- Identified the metal and alloy powders that are able to meet manufacturing and component durability requirements.
- Identified and standardized the performance test methods.
- Identified the testing instrumentation to characterize the metal powder properties.
- Identified all the P/M techniques to process auto parts (production, mixing/blending, cold and warm compaction, sintering, heat treatment, optional finishing operations, etc.).
- Identified the existing numerical techniques for simulating P/M forming processes.
- Identified the important parameters that influence the compaction processes.
- Identified and evaluated the existing powder material models that will simulate P/M compaction processes.

- Developed a constitutive law based on the Modified Drucker-Prager cap model mixed with the microstructure-based plasticity model to predict the material state during compaction. The model is composed of several material parameters that are density-dependent.
- Developed an algorithm to implement the compaction constitutive model into the finite element code ABAQUS/Explicit using the user material subroutine VUMAT.
- Defined a powder metallurgy test matrix, which will be used to create a microstructure-property database for validation of model constants and accurate prediction of powder mechanical behavior.
- Performed Finite Element Analysis on 3D cylinder, gear and main bearing cap with virtual material parameters, geometries and tool motions to illustrate the capability of the model for simulating powder compaction of automotive components.

Future Direction

- Perform microstructural evaluations and mechanical property tests on P/M cylinder geometry to determine microstructure-property relations during compaction, sintering, and in-service duty life. With the above software developed, the model will be correlated to these microstructure-property relations.
- Determine the interparticle friction coefficient, using a simple Coulomb law of friction by measuring the tangential forces at the contact surface and determine the influencing parameters contributing to the friction effects.
- Perform atomistic simulations for different diameter particles (3.52 nm, 7.04 nm, and 14.08 nm) with a BCC particle arrangement with periodic boundary conditions to examine the effect of particle size on the density distribution of the sample after compression.
- Develop algorithm and implement the developed compaction model into the finite element code ABAQUS/Standard to predict the springback of a compacted part during ejection.
- Modify the existing sintering model from Pennsylvania State University to insert internal state variables and link it to the compaction model. Develop algorithm and implement the sintering model in ABAQUS/Standard
- Predict the material state during the powder compaction and sintering processes with the developed math-based models for a main bearing cap and gear.
- Validate process model (including tool geometry, friction, tool and metal temperatures, die rate and pressure) and property models on P/M bearing cap and gear with experiments.
- Document the progress by writing final reports for the second year project by October 31, 2006.

Introduction

In October 2004, the Computational Manufacturing and Design Department at the Center for Advanced Vehicular Systems (CAVS) started the Powder Metallurgy Performance project with the guidance from the Big Three automakers (General Motors, Ford and DaimlerChrysler), and the Center for Powder Metallurgy Technology of North America (CPMT). The project employs the accomplishment of a previous USAMP Lightweight Metals Group project where a microstructure-based plasticity material model has been able to capture the plasticity and damage effects for A356 aluminum and AM60 magnesium, and where it was shown that the model can be used to optimize a control arm made of this latter material [Horstemeyer et al., 2002]. Using the same methodology, the objectives and benefits of this current project are (1) cost reduction (eliminating tooling iterations and prototype components), (2) shortening the lead-time from the concept to implementation for new components, (3) optimization of current components for increasing performance and reducing weight, (4) the availability of modeling tools to evaluate material substitution in components, and (5) the improvement of our scientific understanding of powder metallurgy.

During the first project year, significant progress was made in the area of simulation where all the

numerical techniques needed to perform multiscale and multistage modeling were identified. Also, the microstructure-based plasticity material model was integrated with the Modified Drucker-Prager Cap Model to capture the plasticity of the powder during compaction. In the area of experimentation, a test matrix was established to build a complete microstructure property database for compaction, sintering, performance and fatigue. The project team is currently looking for industrial partners to provide iron and aluminum powders and specimens to CAVS, and also to perform experiments using equipment that is not available at CAVS site.

P/M Manufacturing Process

Powder metallurgy, or P/M, is a process for forming metal parts by compacting and heating metal powders to just below their melting points. Although the process has existed for more than 100 years, over the past quarter century it has just become widely recognized as a robust process for producing high-quality parts for a variety of important applications. This success is due to the advantages the process offers over other metal forming technologies such as forging and metal casting, advantages in material utilization, shape complexity, near-net shape dimensional control, among others [German, 1994]. In reality, P/M comprises several different technologies for fabricating semi-dense and fully dense components. In this project, we will study the conventional P/M process, referred to as press- and-sinter, which is used to make the two automotive parts, gear and bearing cap.

In this conventional process, P/M parts are formed by a sequence of processes. The first few steps are the selection of suitable powder forms, the production of powders, and the weighing and mixing of them. The blended powders are then pressed or compacted into a desired shape in a tool set, consisting of punches, a die and core rods. The green compacts are then sintered. To improve the properties of the sintered products, finishing operations may be carried out.

Mixing/Blending

The blending of metal powder, which is done under controlled conditions (i.e., air, inert atmosphere, or liquid) to avoid contamination and deterioration, fulfills several purposes:

- Produces a uniform distribution of particle sizes and shapes.
- Allows different metals to be mixed to obtain specific physical properties.
- Improves metal powder interaction and prolongs the life of dies used when metal powder is blended with lubricant.

Compaction

Powder compaction is the most critical stage in the P/M manufacturing process. During this operation, the blended powder undergoes significant dimensional changes as the powder height is reduced. The powder is compacted to form the shape of the desired part. The density after compaction (also called green density) depends on the compaction pressure, dimensions of the compacted part, tooling motions and powder yield strength.

Sintering

Sintering follows the process of compacting and shaping the powdered material. After compaction, the strength of the material is low. Sintering, then, increases both the physical and mechanical properties of the material. Sintering is the process of heating the material to a temperature below the melting temperature but high enough to allow bonding or diffusion among the individual particles. Continuous sintering furnaces are used for most production. These furnaces have three chambers:

- A chamber to volatilize the lubricants in the green compact in order to improve bond strength and prevent cracking. It is called the burn-off chamber. It slowly raises the temperature of the compound in a controlled manner.
- A high-temperature chamber for sintering. It is the site of actual solid-state diffusion and bonding between the powder particles. The time during the second stage of sintering must be sufficient to produce the desired density and final properties.
- A cooling chamber.

The furnace thermal profile should be properly controlled to obtain successful sintering and optimum properties. During the sintering process a wide variety of physical, chemical, and metallurgical phenomena occurs within the mass of metal powder

particles. These phenomena are influenced by the sintering conditions, such as time, temperature, and atmosphere, and the chemical composition of the powder mass.

Finishing Operations

Finishing operations are usually performed after sintering. For better dimensional accuracy, different machining operations such as coining and turning are performed. Heat treating (quench and temper, steam treat) the sintered part will improve its strength, hardness, and wear resistance. Finishing operations are also performed to improve the surface characteristics of the part.

Numerical Methods for P/M Modeling

To perform the modeling of automotive P/M parts, the P/M manufacturing process can be divided into a number of distinct stages: powder transfer, powder compaction, ejection, sintering and heat treatment. Different numerical techniques and constitutive laws can be used for modeling these stages of the P/M process. Linking the different models is a requirement to synthesize the whole P/M process and to make the procedure history-dependent (Figure 1). Using multiscale methods and techniques for bridging scales from atomistic to continuum can be very helpful in understanding the fundamental relationship between microstructure and important macroscopic materials properties [Horstemeyer and Wang, 2003]. In this project, the numerical techniques considered are Molecular Dynamics, the Finite Element Method and eventually the Discrete Element Method.

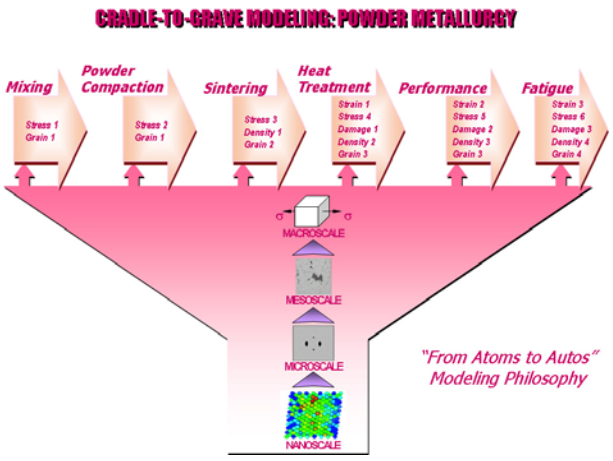

Figure 1. Cradle-to-Grave modeling of P/M process.

Molecular Dynamics

The molecular dynamics method was first introduced by Alder and Wainwright in the late 1950's [Alder and Wainwright, 1957 and 1959] to study the interactions of hard spheres. At the nanoscale level, Molecular Dynamics techniques address the response of individual atoms under mutual interactions. Due to the limitations imposed by computer speed and memory, the total number of atoms is of the order of a couple of millions and the total real time of simulation is of the order of picoseconds. Molecular Dynamics simulations are considered here as 'numerical experiments' to quantify the appropriate cause-effect relations between the microstructure and the mechanical properties for P/M compaction, sintering, and sizing processes at the macroscopic level. By varying packing arrangement (Figure 2), nanoparticle size and compacting temperature, we can understand the deformation and diffusion mechanisms which occurred in an assembly of the particles, such as dislocation slip, diffusion through dislocations, grain boundary sliding, interparticle friction and void/crack nucleation during the P/M consolidation process.

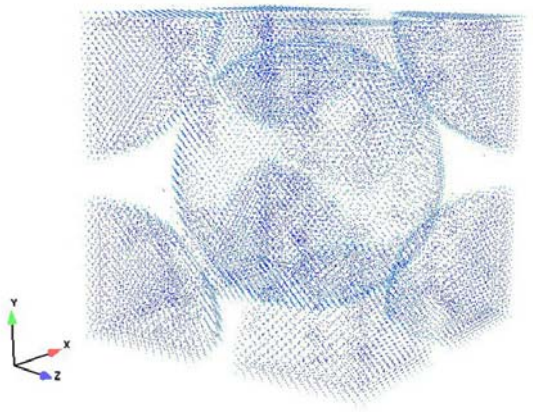

Figure 2. Molecular Dynamics – Nanoscale simulations of powder compaction with BCC packing configuration

The macroscale internal state variable constitutive theory can then be correlated and validated with these atomistic simulations of nanocrystalline powder to quantify the level of influence by these material parameters: inter-particle friction, length scale effects and particle size effects. These results associated with the experimental database constitute part of the effort to build comprehensive microstructure-property relationships of the P/M process.

Discrete element analysis

Discrete element methods (DEM), also known as distinct element methods, were first developed for granular materials by Cundall and Strack [1979]. It has been mainly applied to soil mechanics and many other researchers have used it for a variety of granular dynamics simulations. It consists of numerical simulations of interacting individual particles that provide significant information on particle motion, and contact forces. To formulate motion equations, the particles are treated as individual entities with Newtonian motion in a gravitational field. This method has been advanced by many researchers and it has been used extensively to study the flow and deformation mechanisms of granular materials.

The purpose of using DEM simulations in this project is to study and improve the flowability of metal powder during mixing, die filling and powder transfer. The DEM model can analyze the sensitivity of the interparticle and particle/die friction coefficients, the geometry of the particles, and the particle size distribution. Therefore, the determination of an apparent density distribution right before the onset of pressing by using DEM simulations should only increase the accuracy of the powder compaction modeling (Figure 3).

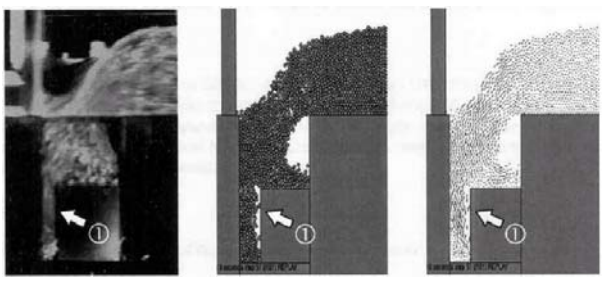

Figure 3. DEM simulation of die filling [Gillia et al., 2002].

Finite Element Method

In recent years, finite element (FE) analysis has received wide attention for its applicability to powder metallurgy (P/M) industry. With a significant level of reliability and proven quality control, these techniques provide a valuable tool in predicting density and stress distributions in the pressed compact prior to the actual tooling design and manufacturing process.

In this project, the finite element method (FEM) is the primary numerical tool for simulating die compaction and sintering, and for design and performance optimization of the P/M automotive parts. By implementing user-defined routines (UMAT and VUMAT) for both compaction and sintering processes into the general purpose finite element program ABAQUS [2003], quantitative predictions of density distributions and shape distortions can be obtained as well as the stresses in the tool components. Further, by employing optimization techniques to the simulation of powder processing steps, the final properties and design of P/M parts can be tailored by specific levels as desired.

Test Matrix and Characterization Method

For constitutive laws to be successful, computer simulation should be accompanied by a complete experimental database. The accuracy of numerical prediction depends on appropriate experimental data to calibrate and validate the powder material model.

In the first phase, a test matrix (Table 1) has been established to perform microstructural and mechanical property tests on P/M specimens so as to determine microstructure-property relations during compaction, sintering, and in-service life performance. As the compaction model is developed and implemented into the finite element code, the next task is to perform closed-die, isostatic and triaxial compaction tests to correlate the model with the microstructure-property relations. Many researchers have observed that the metal powder material model can be improved by updating the elastic and plastic properties (elastic moduli, cap eccentricity, material cohesion, internal friction, green strength) with the relative density $\tilde{\rho}$.

Table 1. Test Matrix for Compaction, Sintering, Performance and Fatigue

	Experiments	Model Calibration
COMPACTION	Determination of Tap Density	Initial Density before compaction
	Closed-die Compaction	Compressibility Curves Cap Hardening parameters for Pressure-Density curve
	Isostatic Compaction	Compressibility curves Cap Hardening
	Triaxial Compaction Isostatic Compaction	Yield Surfaces (density dependent) Cap Eccentricity parameters
	Elastic Properties of compacted powder at different density level	Density-Dependent Elastic parameters Young's Modulus E(r) Bulk modulus K(r)
	Measurement of Internal and die-wall friction	Friction parameter β as function of density
SINTERING	Sintering	Heat Transfer Mass and Dimensional changes Densification Phases
PERFORMANCE	Monotonic Tension Monotonic Compression Monotonic Torsion	Mechanical Properties at different densities of post-sintered P/M parts
FATIGUE	Uniaxial Fatigue Mean Stress Bauschinger Effect	Fatigue Life at different densities of post-sintered P/M parts

For example, the elastic Young's modulus E and the bulk elastic modulus can be deduced from the tests as a function of the density, and the Poisson's ratio can be derived from these two moduli [Pavier and Doremus, 1999]. Figure 4 shows variations of these two moduli with respect to the density (g/cm^3) for an iron-based powder. The Young's modulus for wrought iron is of the same order of magnitude (210 GPa) as the bulk modulus (175 GPa). Therefore, under high compressive stresses the powder has an elastic-plastic behavior similar to its constituent material. Also, the failure line, which is assumed to be linear in the model, can be determined by measuring the green strength in at least two test configurations with different stress triaxiality, such as the compression test, the Brazilian disc test, and the four-point bending test [Coube and Riedel, 2000]. Isostatic compaction is needed to determine the compressibility curves (density versus hydrostatic compacting pressure). More expensive triaxial tests are necessary to determine the shape of the cap. It is expected that exact knowledge of the cap curvature may have a minor influence on the final density distribution in most practical cases. In special cases, however, when a considerably profiled upper punch intrudes into the powder, the shape of the cap can influence the predicted density distribution significantly, so that more reliable values of the eccentricity parameter are needed. In addition, friction measurements should be performed, especially if simulations of slender parts are intended, Fig. 5.

Recently, Coube and Riedel [2000] allowed the material parameters, internal friction μ and material cohesion d, to be internal state variables and they are functions of both volumetric and equivalent plastic strain rates, Figure 6. The evolution equations of these variables exhibit a more pronounced softening on the failure line. Note that the objective of this formulation is to describe the cracking as a process of strain localization.

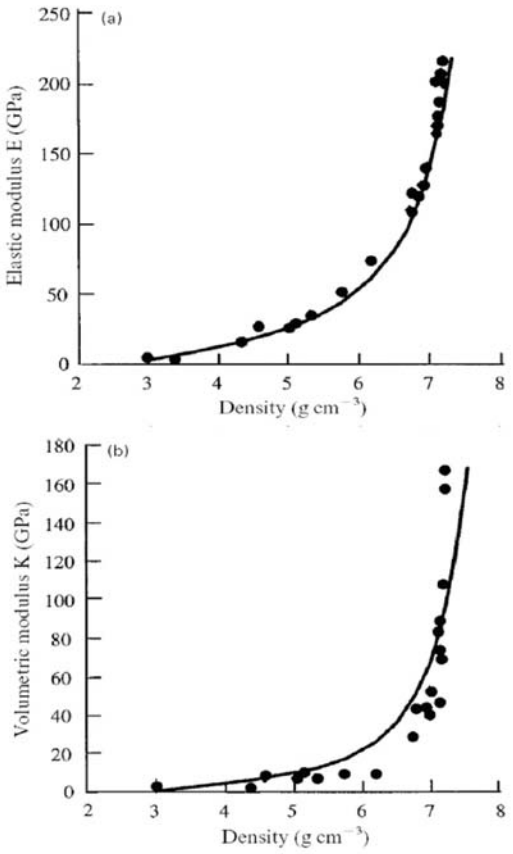

Figure 4. Evolution of given elastic moduli as function of density [Pavier and Doremus, 1999].

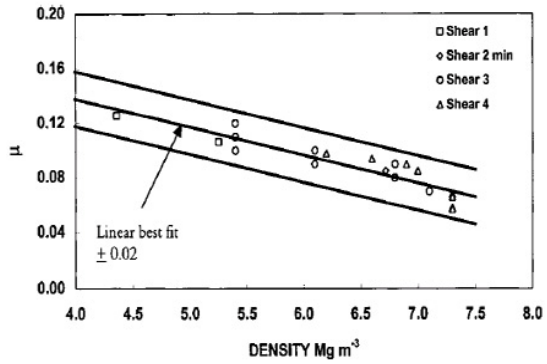

Figure 5. Measurement of internal friction [PM Modnet Methods & Measurements Group, 2000]

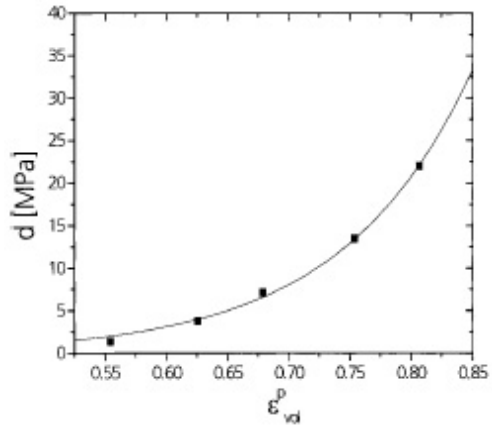

Figure 6. Cohesion strength d versus plastic volumetric strain [Coube and Riedel, 2000]

Modeling of Powder Compaction

The powder compaction is the most critical stage in the Powder Metallurgy (P/M) manufacturing process. Final part density, homogeneity, and strength are highly affected by this crucial operation. According to Khoei and Lewis [1998], a successful model for powder compaction process should reflect the frictional and compressible-densification yielding characteristics of the powder. A powder compaction model also needs the ability to describe the evolution of the porosity or density and the plasticity of the ductile metal particles subject to complex-shape geometries under multiaxial stress states. The density distribution is dependent on the combination of many factors such as geometrical shape, mechanical properties of the powder, and powder-tool frictional behavior.

In order to formulate a physically-based constitutive model, we need to distinguish the importance of three different scales during the deformation processes:

- the deformation of the powder aggregate idealized as a continuum – the classic macroscopic level,
- the deformation of the individual particles – the particle or microscopic level,
- the nanoscale dislocation mechanisms and the interparticle reactions.

Therefore, to have an accurate description of the different scales for metal powder analysis, the material model needs to reflect the following properties as defined by Trasorras et al. [1994], to accurately describe the following:

- Elastic deformation of the powder aggregate
- Plastic deformation of the powder aggregate
- Geometric hardening of the powder aggregate as a result of densification and a very large reduction in volume
- Plastic deformation of the particle according to the behavior described by classical plasticity with isotropic hardening as the powder aggregate is compacted
- Strain hardening of the particle.

In this project, the proposed compaction model consists of mechanical constitutive equations of the plastic deformation of the powder aggregate and the deformation-induced hardening of the particles. The structure of the constitutive equations of a porous material reflects volumetric inelastic deformation and marked pressure dependences. The macroscopic continuum framework assumes the porous medium as a macroscopically equivalent, isotropic, homogenous continuum with the relative density (or void volume fraction/damage) as a scalar internal variable. The anisotropic effects due to orientation and shape of the grains or voids are assumed to be small and are neglected at this moment.

Many mathematical models have been proposed for simulating the behavior of metal powders during rigid die compaction. For the case of macromechanical modeling of the metal powder compaction, the Cap model is one of the most popular constitutive models. The Cap model was originally developed to address the effects of stress state on geological types of materials such as sand, rock, and concrete. It was then adapted for ceramic and hard metal powders and most recently, for ductile metal powders [Gurson and Posteraro, 1994]. Such a model may be directly used for ceramic powders and the like. However, most metal powder compaction operations deal with ductile powders, and the Cap model suffers from a limited ability to incorporate the material property changes in ductile metal particles that accompany densification and deformation of the powder mass. Therefore, to allow hardening of the failure shear envelope, the model should then correlate the hardening of the overall aggregate with the plastic hardening of the particles and the relative density of the compact.

During the powder compaction process, large material rotations and deformation occur. To describe the deformation of ductile metal particles, an internal state variable (ISV) plasticity model is used [Bammann, 1990; Bammann et al., 1993]. The evolution equations for these state variables are motivated from dislocation mechanics and their use enables the prediction of strain-rate history and temperature history effects. The assumption of linear elasticity can be written

$$\underline{\sigma} = \underline{\underline{C}}(\rho) : \underline{\varepsilon}^{e} \tag{1}$$

where $\underline{\underline{C}}(\rho)$ is the elastic stiffness function of the relative density ρ, $\underline{\varepsilon}^{e}$ the elastic deformation, and $\underline{\sigma}$ is the Cauchy.

To characterize the behavior of the powder aggregate, we use a Modified Drucker-Prager/Cap material model. This double surface plasticity model consists of an elastic region in stress space, bounded by a friction-failure line F_s in the low-pressure region, and an elliptic yield cap F_c in the high-pressure region. The mechanical behavior of powders in compression can arise from adhesion and frictional sliding at particle interfaces, fracture of particles, and plastic deformation of particles. Because the metal powder is considered as a ductile material, the yield cap is also influenced by plasticity.

To reduce the conditional branching in the algorithm and to avoid numerical instabilities, a smooth function is introduced to replace the corner intersection between the two surfaces associated with the cap model, i.e., the failure envelope and isotropic-hardening cap surfaces of the Drucker-Prager/Cap model originally proposed by DiMaggio and Sandler [1971]. The modified Drucker-Prager failure surface of the smooth cap model is defined as:

$$F_s = \left|\underline{\sigma} - \underline{\alpha}\right| - F_e(p) = 0 \tag{2}$$

with

$$F_e(p) = d + p\tan\beta - F_p(p) \qquad (3)$$

where β is the material's angle of friction and d is its cohesion strength; $\underline{\alpha}$ is the kinematic hardening tensor; p is the first invariant of the stress tensor $\underline{\sigma}$. The deviatoric stress tensor, $\underline{s}$, is defined as

$$\underline{s} = \underline{\sigma} + p\underline{I} \qquad (4)$$

The hydrostatic stress, p, is written as:

$$p = -\frac{1}{3} I_1 \quad \text{with} \quad I_1 = \text{trace}(\underline{\sigma}) \qquad (5)$$

Following standard conventions in soil mechanics, compression and compaction are assumed to be positive. The key modification to connect the failure yield surface smoothly with the cap yield surface is to include another function F_p in the failure yield surface F_s. The pressure dependent function F_p is here defined by:

$$F_p(p) = H(p - p_c)\left[\frac{p - p_c}{p_a - p_c}\right]^{p_a - p_c} \tan\beta \qquad (6)$$

where p_a is the hardening parameter, $H(\cdot)$ is the Heaviside function:

$$H(p - p_c) = \begin{cases} 1 & \text{if } p \geq p_c \\ 0 & \text{if } p < p_c \end{cases} \qquad (7)$$

The variable p_c is defined by:

$$p_c = p_a - p_d \qquad (8)$$

where p_d is a material parameter.

The cap yield surface has an elliptical shape with constant eccentricity in the meridional $|s\text{-}\alpha|$–p plane (Figure 7). The cap surface hardens or softens as a function of the volumetric plastic strain: volumetric plastic compaction (when yielding on the cap) causes hardening, while volumetric plastic dilation (when yielding on the shear failure surface) causes softening. The cap yield surface is written as

$$F_c = \sqrt{|s - \alpha|^2 - \frac{1}{R^2}[p - p_a]^2} - F_e(p_a) = 0 \qquad (9)$$

with $$F_e(p_a) = d + (p_a - 1)\tan\beta \qquad (10)$$

where R is a material parameter called the cap eccentricity that controls the shape of the cap. The cap hardening variable p_a is an evolution parameter that represents the volumetric plastic strain-driven hardening/softening.

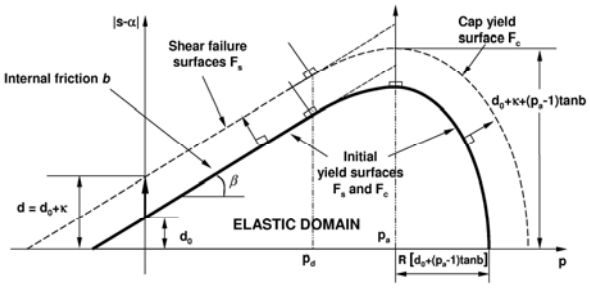

Figure 7. Modified Drucker-Prager/Cap Model: yield surfaces in the |s-α|–p plane

The evolution parameter p_a is a hardening parameter that controls the motion of the cap surface, and p_b defines the geometry of the cap surface. The ellipticity of the cap surface is determined by the material parameter R that relates the hardening parameter p_a to p_b through the relation

$$p_b = p_a + RF_e^*(p_a) \qquad (11)$$

with

$$F_e^*(p_a) = d_0 + (p_a - 1)\tan\beta \qquad (12)$$

where d_0 is the initial material cohesion. Because the ellipticity of the cap surface may also be influenced by the incompressible plasticity, the cap hardening evolution does not take into account the increase in the material cohesion d due to the isotropic plasticity of the particle.

Sandler and Rubin [1979] proposed a relationship to define the evolution of the cap's motion, which is defined by the isotropic cap hardening rule

$$\bar{\varepsilon}_{vol}^{p} = W\left(1 - \exp\left[-c_1 p_b^{c_2}\right]\right) \qquad (13)$$

In which W is the maximum plastic volumetric strain (at hydrostatic compression *'lockup'*), c_1 and c_2 are material shape factor parameter, and $\bar{\varepsilon}_{vol;}^{p}$ is the effective volumetric plastic strain defined by integrating

$$\dot{\bar{\varepsilon}}_{V}^{p} = \begin{cases} \dot{\varepsilon}_{vol}^{p} & \text{if } p_a > 0 \text{ and } I_1 > 0 \\ 0 & \text{otherwise} \end{cases} \qquad (14)$$

where ε_{vol}^{p} is the plastic volumetric strain. The density can also be defined by an associative or a non-associative flow rule with pressure dependent deviatoric [Marin and McDowell, 1996].

The form of the elastic domain is defined in terms of the failure shear and cap yield surfaces as

$$F_s(|s|, p) < 0 \quad \text{and} \quad F_c(|s|, p) < 0 \qquad (15)$$

For multisurface plasticity, an appropriate statement of the flow rule relies on Koiter's generalization, which, using the flow potentials F_s and F_c, takes the form

$$\underline{\dot{\varepsilon}}^{p} = \dot{\gamma}_s \frac{\partial F_s}{\partial \underline{\sigma}} + \dot{\gamma}_c \frac{\partial F_c}{\partial \underline{\sigma}} \qquad (16)$$

where $\dot{\gamma}_S$ and $\dot{\gamma}_c$ are the plastic consistency parameters. Plastic loading or elastic loading/unloading is formulated in Kuhn-Tucker form by means of the relation

$$\dot{\gamma}_s, \dot{\gamma}_c \geq 0, \; F_s, F_c \leq 0 \text{ and } \dot{\gamma}_s F_s + \dot{\gamma}_c F_c = 0 \qquad (17)$$

The plastic hardening of the particles allows the hardening of the failure shear envelope and the cap surface. The cohesion of the powder aggregate d will then increase as follows

$$d = d_0 + \kappa + V(\theta)\sinh^{-1}\left[\frac{\dot{\bar{\varepsilon}}^{p}}{f(\theta)}\right] \qquad (18)$$

The cap hardening evolution is based on the material cohesion d_0 and is then not affected by the dilatancy of the cap surface due to particle hardening of particles. The material cohesion d_0 is given by

$$d_0 = d_1 \exp\left[d_2 \bar{\varepsilon}_{vol}^{p}\right] \qquad (19)$$

In Figure 8, we observe the evolution of the cap yield surface during densification where only the plasticity of the powder aggregate is considered (no deformation of individual particles) and the cap eccentricity R is function of the density as follows

$$R = \frac{R_1 - R_2}{1 + \left(\rho / \rho_c\right)^{k}} + R_2 \qquad (20)$$

where d_1, d_2, R_1, R_2, ρ_c and k are material parameters.

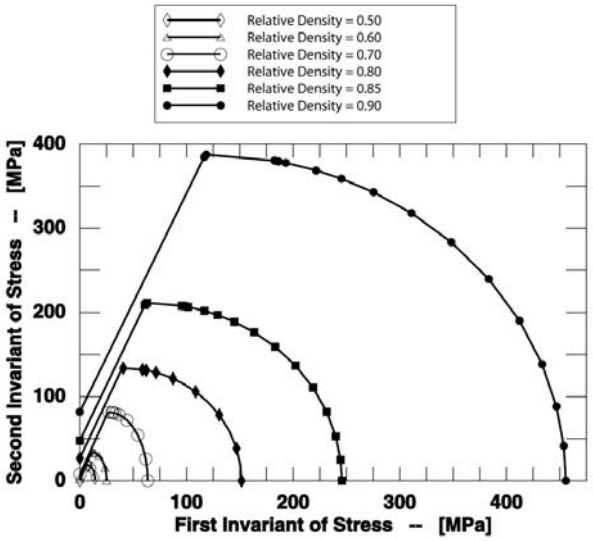

Figure 8. Evolution of the cap yield surface during densification.

Fundamental: Nanoscale Friction Analysis

The Molecular Dynamics research is focused on modeling the interparticle behavior between two nanoparticles during compression for friction analysis. Each particle is conveniently represented by a sphere. Nickel is chosen as the powder material since nickel particles are spherical and its Embedded Atom Method (EAM) potential is already defined. The purpose of this nanoscale analysis is to study the interparticle friction for different lattice orientation and particle packing configuration, and to understand its influence on macroscopic material properties.

Atomistic simulations using EAM potential were performed for various model setups, as shown in Figure 9. The model setups consisted of two contacting particles of various sizes, crystal orientations, and misorientation angles to analyze the effect of these parameters on nanoparticle behavior. Boundaries were defined as free surfaces in the *x*- and *z*-directions, and by applying a compressive load along the *y*-direction by defining an applied velocity. The imposed velocity resulted in very high strain rates, on the order of $10^8\ s^{-1}$.

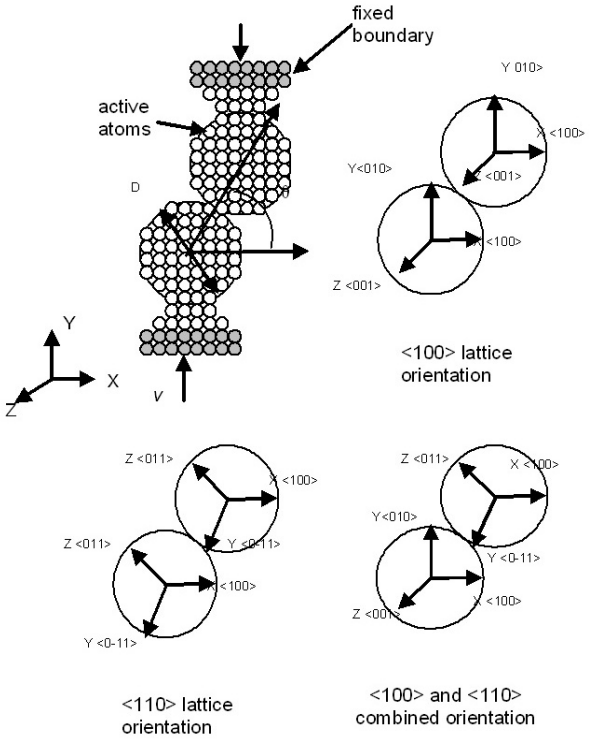

Figure 9. Model configuration with θ=30°, 60°, 90°, D = 3.52 nm, 10 nm, 20 nm, applied velocity v = 0.022 *Å/ps*, and various crystal orientations.

Before the velocity is applied, a Nose-Hoover thermostat was used to enforce a constant temperature of 300 K, and to equilibrate the system accommodating any surface relaxation the system may have. At the completion of the equilibrium phase, a linear *y* velocity profile $v_y = \dot{\varepsilon} y$ is applied to all atoms. This is done in order to avoid an initial shock wave, which otherwise would result from the instantaneous application of the boundary conditions on the $\pm y$ surfaces. Figure 10 shows the model configuration for the various particle sizes investigated in the analysis. These results were after 10 psec of temperature equilibrium, but prior to the applied velocity.

Figure 11 shows stress-strain results from the molecular dynamics simulation for two 3.52 nm particles at 30 degree misorientation angle. Each dot in the figure represents an individual nickel atom with a centrosymmetry value, a measure of an atom's disturbance for its crystalline lattice position, greater than 2.0. Several locations of micro-yield, where the stress-strain behavior deviates from elastic linearity, were identified on the curves.

The first location of micro-yield was when the initial dislocations were emitted from the grain boundaries. The steep drops in the stress-strain response were due to the formation of shear bands. Size effects on the axial stress strain results show that as particle size increases, the yield strength decreases, which is consistent with experimental results. Misorientation angle effects on the axial stress-strain response result in the highest yield stress for the 90 degree case and smallest yield stress for the 30 degree case. Lattice orientation effects on the axial stress-strain response show the most severe shear band formation occurred on the <110> crystal orientation.

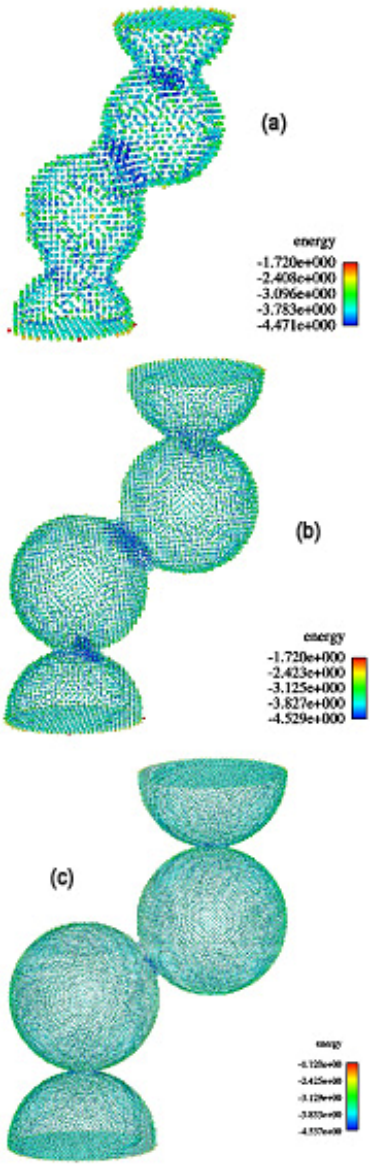

Figure 10. Atomistic model for (a) 3.52 nm (2123 atoms per particle), (b) 7.04 nm (16757 atoms per particle), and (c) 14.08 nm diameter particles (134000 atoms per particle), after 10 ps of temperature equilibrium and no applied velocity.

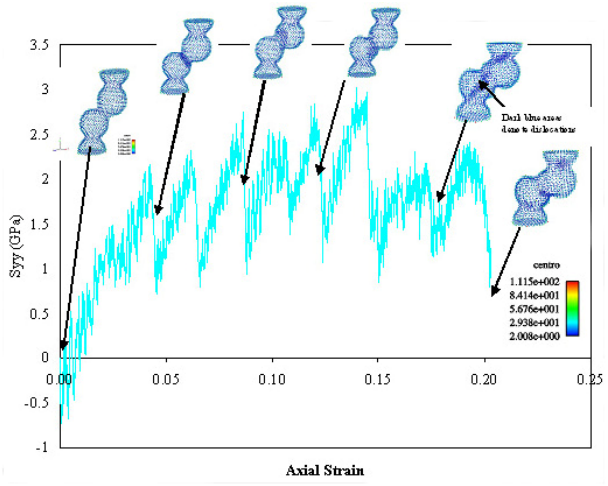

Figure 11. Compressive stress vs. Axial strain results for 3.52 nm particles with <100> crystal orientation at 30 degree misorientation angle during compression with 5E8/s applied strain rate.

Application: FE Analysis of Compaction

In order to illustrate the applicability of the developed compaction model, the powder behavior during the compaction of a set of complex forming processes are analyzed numerically in ABAQUS/ Explicit. Two different geometries have been selected; a 3D cylinder and a gear. Simulations of the 3D cylinder will be used in the second phase for correlation and validation of model constants, and the gear and bearing cap are the two chosen automotive components for durability, quality control, performance and design optimization.

The two geometries were simulated by using displacement control when increasing the punch movement. The parameters were chosen arbitrarily and do not really represent any existing metal powders. Numerical results presented in this section do not reflect any experimental data or results in the literature. The goal is to illustrate how the model can capture the density distributions during compaction. In both analyses, the dies were represented by rigid bodies and a friction coefficient of value 0.1 was applied at the interface powder/die. The upper and lower punches were moving at the same speed and in opposite directions. The theoretical density is 7.8 g/cc and the initial density is equal to 4.13 g/cc, which represents 53% of the theoretical density.

The 3D cylinder was set with initial height of 100 mm before compaction, the diameter was

12.5 mm. Figure 12 shows the relative density distribution after compaction, which corresponds to a height of 60 mm. It is noteworthy that the neutral zone is located at the center of the cylinder and on the lateral surface, and the highest relative density (93%) is at the end surfaces on the corner next to the die wall. The density gradient along the cylinder axis is due to the die wall friction. Figure 13 shows the compressibility curve of a given point.

The inner, root and outer diameters of the gear were respectively 8 mm, 20 mm and 27 mm, the thicknesses before and after compaction were 8 mm and 4.8 mm (Figure 14). Note that the behavior of density gradient along the gear axis and next to the die wall or core rod is the same as that in the

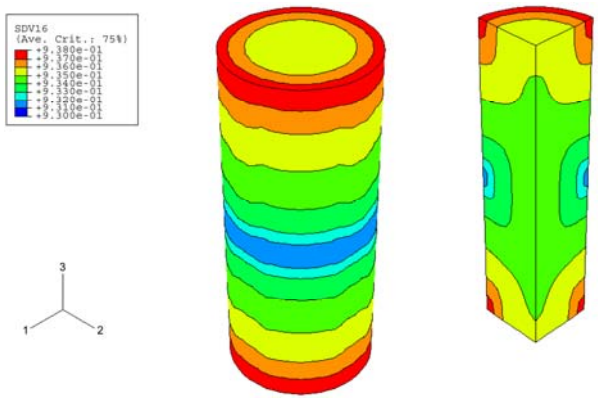

Figure 12. Relative density distribution in a 3D cylinder.

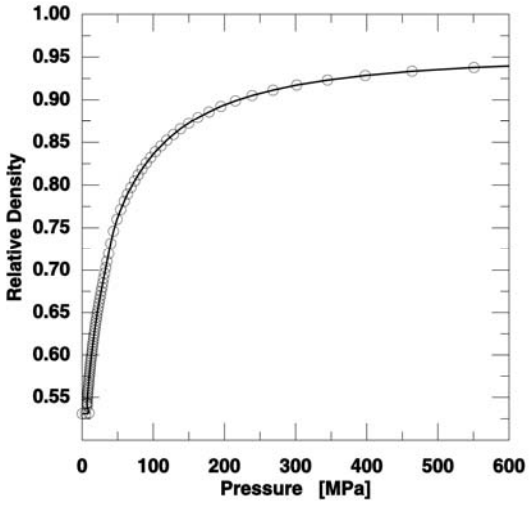

Figure 13. Compressibility curve.

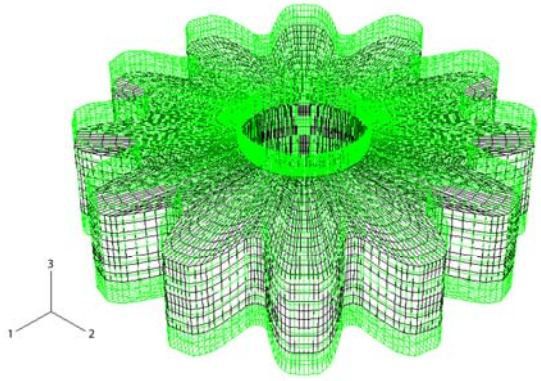

Figure 14. Undeformed and deformed meshes of a gear.

cylinder case before due to the die wall friction. The highest density (7.3 g/cc) is at the gear tooth arcs, next to the die wall and the punches, and at the inner diameter, next to the core rod. The density distribution between the inner and root diameters is mostly homogeneous due to the relative small thickness of the gear.

In the next year effort, we will focus on the comparison between numerical simulations and experimental validations of gears and bearing caps.

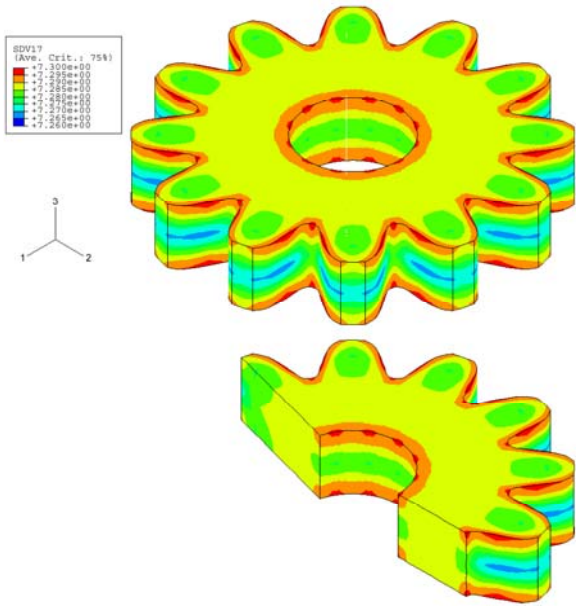

Figure 15. Density distribution in a gear (g/cc).

Conclusions

The Powder Metallurgy Performance Modeling of Automotive Components Project has made significant progress especially in the area of modeling where a constitutive law to predict material state during powder compaction was developed and implemented into a finite element code. This constitutive model is based on the Modified Drucker-Prager cap model and mixed with the microstructure-based plasticity. It also includes different density-dependent material parameters. Other project accomplishments include identification and standardization of performance test methods; identification of testing instrumentation to characterize the metal powder properties; establishment of a test matrix to build a complete microstructure property database for compaction, sintering, performance and fatigue. In fiscal year 2006, the project team expects to conduct experiments on powder compaction defined in the test matrix, complete sintering modeling and link that model to the compaction model, perform atomistic simulation to determine the interparticle friction coefficient, and finally write a documentation report of the second phase of the project in October 2006.

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Presentations/Publications/Patents

1. "Design of Powder Metallurgy Components Considering History and Multiscale Effects," H.I. Sanderow, P. Wang, Y. Hammi, T.Y. Stone and M.F. Horstermeyer, presented at the 2005 MPIF Fall Management Conference and 61st Annual Meeting, October 11, 2005, Key Biscayne, Florida.
2. "Constitutive Modeling for Powder Compaction and Densification," Y. Hammi, T.Y. Stone and M.F. Horstermeyer, presented at the PM^{2}TEC 2005 International Conference on Powder Metallurgy & Particulate Materials, June 21, 2005, Montreal, Canada.
3. "Constitutive Modeling of Metal Powder Behavior during Compaction," Y. Hammi, T.Y. Stone and M.F. Horstermeyer, presented at the SAE 2005 World Congress, April 12, 2005, Detroit, Michigan.

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