Modelling of PM Processing

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Outline

✓ Introduction: interest of modelling and pertinent scales

✓ Discrete element modelling at particle assembly scale method examples

✓ Finite element analysis at component scale method examples focus on multimaterials and field assisted sintering

✓ Summary
Interest of modelling

Support for understanding
• Analysing observed phenomena
• Validating assumptions drawn from experiments
• Guiding novel experiments
• Anticipating the effect of material and process parameters, etc.

Tool for virtual processing
• Prediction of material behaviour during an industrial process for reducing trial and error procedure

For each problem, the most relevant scale should be identified.
At each scale, specific issues can be investigated and various modelling techniques are available.

This lecture focuses on two scales, particle assembly and component, and two techniques, discrete element method and finite element analysis.
Particle assembly scale

Related issues:

- Volume changes
- Grain growth
- Cracking
- Properties (conductivity, permeability, ...)

Induced by individual and collective behaviour of particles in thermo-mechanical conditions

Modelling techniques:

- Discrete Element Method
- Monte Carlo models
- Finite elements analysis
Discrete Element Modelling (DEM)

Principle:

Simulating an assembly of particles (typically thousands) in a box, assuming an interparticle contact law, imposing force or displacement at the boundaries of the box and solving the equations of motion for every particle.

DEM codes:

PFC (commercial), EDEM (commercial), SimPARTIX (Fraunhofer Freiburg), dp3D (SIMAP/Univ. Grenoble Alpes), etc.
Typical process of a DEM simulation

- Contact detection + calculation of contact forces (Normal + Tangential) with a prescribed contact law
- Calculation of the total force applied to each particle
- Calculation of accelerations due to applied forces (same procedure for rotations)
- New positions of particles, quasi-static simulations

$$\ddot{x} = \frac{F}{m} \rightarrow \dot{x} \rightarrow x$$

final position after rearrangement
Example of DEM simulation (1)

Die filling

Relative density at various step of the filling process

aggregate mimicking a Distaloy AE particle

Contact law:
Elasticity and adhesion (JKR model)
Aggregates cannot break.

Bierwisch et al., Powder Tech. 196 (2009) 169
Example of DEM simulation (2)

Pressing of particle aggregates

Contact laws:
- Intraaggregate: elasticity and breaking
- Interaggregate: adhesion (JKR model)

Experiments:
Example of DEM simulation (3)

Sintering of copper powder with grain growth

**Contact law**: Two-sphere sintering equation with overlapping volume redistribution

- Relative density 0.64
- 4000 particles

![Image of copper powder microstructure]

- T = 850°C
- T = 950°C

**Graph**:
- Densification rate, 1/s
- Relative density

**Legend**:
- DEM with constant particle size
- DEM with coarsening
- Experimental data

Example of DEM simulation (4)

Sintering of a ceramic powder upon a rigid substrate

→ Constraint sintering

Contact law: Two-sphere sintering equation

*Martin and Bordia, Acta Mater. 57 (2009) 549*
Example of DEM simulation (4)

Sintering of a ceramic powder upon a rigid substrate

Formation of defects close to the substrate

*Martin and Bordia, Acta Mater. 57 (2009) 549*
Component scale

**Pertinent issues:**
- Shape changes
- Heterogeneities in density, microstructure or composition
- Cracking

Due to powder-die friction, component geometry, gravity, thermal gradients, etc.

**Modelling technique:**
- Finite element analysis

The material is considered as a *continuum*. 
Finite element analysis

- Experimental data
- Assembly-scale modelling

Constitutive equation

Initial state: dimensions, density distribution, residual stresses

Process conditions: pressure, temperature, boundary conditions ...

Finite element simulation

Deformation, density distribution, stresses, etc., all over the process
Relation describing the deformation of an *elementary volume* of material under « any » temperature and stress conditions met during processing:

\[ \dot{\varepsilon} = F (\sigma, \dot{\sigma}, T, \text{internal variables}) \]

- \( \dot{\varepsilon} \): strain rate tensor
- \( \sigma, \dot{\sigma} \): stress and stress rate tensors
- \( T \): temperature (if required)
- internal variables: relative density \( D \), grain size \( G \), etc.
Constitutive equations for powders

<table>
<thead>
<tr>
<th>Process</th>
<th>Mechanisms</th>
<th>Class of equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressing</td>
<td>Rearrangement, Plastic deformation</td>
<td>Elasto-plastic, granular-type</td>
</tr>
<tr>
<td>Sintering</td>
<td>Atom diffusion</td>
<td>Viscous, with a term accounting for free sintering</td>
</tr>
</tbody>
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Several commercial FEA codes integrate constitutive equations for powder pressing but none for sintering.
Example of FEA simulation (1)

Pressing and sintering of a WC-Co cylinder

Friction

→ Green density gradients

→ Conical shape

Compression force

Relative density after simple action pressing

Geometry and relative density after sintering

Powder-die friction

Powder/punch friction
Example of FEA simulation (2)

Pressing and sintering of an alumina part

Green Sintered

Pressing

Shape changes after sintering

Densité relative
1: 0.560
2: 0.575
3: 0.590
4: 0.605
5: 0.620
6: 0.635
7: 0.650
8: 0.665
9: 0.680
10: 0.695
11: 0.710

Relative density after pressing

Example of FEA simulation (3)

Sintering of a WC-Co rail

Green density distribution after die pressing

Bending during sintering

O. Gillia, PhD. Thesis, Grenoble, 2000
Multimaterials (1)

Sintering of a two-material part

“Metcer”
Metallic phase is preponderant

“Cermet”
Ceramic phase is preponderant

Different sintering behaviours

→ What about co-sintering?
Multimaterials (2)

In situ observation of shape changes

Crack formation during heating

Finite element simulation

Vertical tensile stress distribution

Field assisted sintering (1)

Phenomena:
Interaction between an electric field and the material
  → Internal heating source
  → Temperature increase
  → Sintering

FEA procedure:
Iterative simulation coupling electrical, thermal and mechanical phenomena
Field assisted sintering (2)

Spark Plasma Sintering


Microwave Sintering

Summary

✓ Modelling can bring relevant information for better understanding and prediction of PM processes.

✓ Various techniques and tools are available for this purpose; the choice depends on the scale of interest and on the issue to be investigated.

✓ Discrete element modelling is particularly relevant for particle assembly scale and finite element analysis for component scale.

✓ Modelling is especially helpful for the investigation of complex processes, as for example multimaterials fabrication, constraint sintering and field assisted sintering.