FINITE ELEMENT MODELING OF FAST

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Outline

- Introduction to FEM for users
- Basic thermo-electric modeling
- Fully coupled model
- Discrete models
- Open issues
THE NEXT FEW SLIDES CONTAIN BLATANT SELF PROMOTION AND MAY BE ILLEGAL IN SOME STATES
RANKED 11\textsuperscript{th} 
OUT OF 88 MATERIALS PROGRAMS 
IN THE 2010 NRC S-RANKINGS

11.3 Faculty Members
1 Lecturer

116 Undergraduate Students

58 PhD Students
70% Domestic
10 PhDs/year awarded for 2004-2010

$5M Annual Research Expenditures

4/11/2011
FACULTY

AREAS OF RESEARCH
Nanomaterials & Nanotechnology
Biomaterials
Electronic and Photonic Materials
Nuclear Materials Science
Materials for Energy
Polymers and Soft Materials
Materials Processing
Faculty Distinctions

- 1 PECASE Awardee (Spanier)
- 3 NSF CAREER Awardees (Zavaliangos, Gogotsi, Li)
- 1 NIH, 1 ARO, and 1 Whitaker Foundation Young Investigator (Marcolongo, Spanier)
- 2 x R&D 100 Awardees (Gogotsi, Taheri)
- Collegiate Inventors Award (Gogotsi)
Faculty Distinctions

- **Fellows:**
  - 2 ACerS (Barsoum, Gogotsi)
  - 2 ASM (Lawley, Knight); 1 ECS, 1 AAAS, 1 MRS (Gogotsi)
  - 1 TMS (Lawley), 2 АΣΜ (Knight, Kalidindi)

- **1 NAE Member** (Lawley - emeritus)

- **3 Alexander von Humboldt Awardees**
  - (Barsoum, Li, Gogotsi)

- **3 Journal Editors** (Gogotsi, Kalidindi, Lawley), and 3 on Journal Editorial Boards (Li, Marcolongo, Zavaliangos)
# RESEARCH THRUSTS

<table>
<thead>
<tr>
<th>Soft materials</th>
<th>Earth-abundant electronic &amp; catalytic materials</th>
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<tr>
<td>- soft materials for biomedical applications</td>
<td>- complex oxide films and heterostructures</td>
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<td>- interfacial phenomena</td>
<td>- ferroic and multi-ferroic materials</td>
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<td>- Soft materials synthesis</td>
<td>- eco-friendly synthesis of quantum dots</td>
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<tr>
<td>- Soft materials for bio-sensing</td>
<td>- eco-friendly growth and processing methods</td>
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</tbody>
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<table>
<thead>
<tr>
<th>Materials at extremes</th>
<th>Nanomaterials for energy &amp; biomedical applications</th>
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<tbody>
<tr>
<td>- materials under irradiation and nuclear materials</td>
<td>- carbon and carbon-derived based materials</td>
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<td>- dynamic microscopy</td>
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<td>- MAX phases</td>
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<td>- carbon nanotube-based celluclar probes</td>
</tr>
<tr>
<td>- coupled phenomena</td>
<td>- nanotubes and nanowires</td>
</tr>
</tbody>
</table>
PhD Student Placement (2007-10)

- **Defense**
  - Wright Patterson Air Force Base
  - Army Research Laboratory (2)

- **National Labs**
  - Los Alamos (2), Lawrence Berkeley, NIST

- **Large companies**
  - Honeywell, United Technologies, FujiFilm, Slumberger

- **Small companies**
  - TBT Group (2), Y-Carbon [Drexel technology licencees]
  - Molecular Biometrics, Ingeni SA

- **Faculty**
  - University of Bath (UK), The College of New Jersey, Çankaya (Turkey)

- **Postdocs**
  - MIT, Yale, ETH, UPenn, Clemson, UConn, Rutgers
Shameless self promotion over
Contributors

Drexel PhD Students:
Jing Zhang (2004, now faculty at U. Alaska)
Brandon McWilliams (2007, now with Army Research Lab)

Prof. Joanna Groza’s group @ UCDavis

Funding: NSF-DMII and ARO/ARL
Simulation of FAST

Pressing

Sintering

Electric current
What is modeling?
What is simulation?
Why model & simulate?

- Access to “information” that cannot be obtained by experiments
- What-if scenarios (scale up, tool design, control algorithm testing)
- Cost minimization by reduction of experiments

Note 1: Models don’t need to be exact (they never will)
Note 2: “Don’t try this at home – I am a trained professional”
FINITE ELEMENTS
an overview for users
LAB CHARACTERIZATION

INDUSTRIAL PROBLEM
Real parts have

- **Complex geometries** that can be the origin of variations in temperatures, stress, properties
- **Complex interactions** with the environment, such as friction, radiation, convection etc. which also may be related to variations in temperatures, stress, properties...
Non-uniform everything...

Analytical solution impossible

Uniform stress & Temperature
straightforward to analyze
(but you can be surprised with the difficulties with a simple test)

2008 IAJC-IJME
International Conference on Engineering & Technology:
Globalization of Technology - Imagine the Possibilities!
November 17-19, 2008 -- Music City Sheraton, Nashville, TN, USA
Numerical Simulation of Pressing and Sintering in the Ceramic and Hard Metal Industry

T. Kraft, O. Coube and H. Riedel
Fraunhofer-Institute for Materials Mechanics
Wöhlerstrasse 11, D-79108 Freiburg, Germany
Instead of ....

We need to solve ......

\[
\sigma_{ij} = E_{ijkl} \varepsilon_{kl}
\]

\[
\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} = 0
\]

\[
\frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} = 0
\]

\[
\frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{zy}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} = 0
\]
Instead of ....

\[ q = kA \frac{d\theta}{dx} \]

We need to solve ......

\[ \nabla (k \nabla \theta) + \dot{q}_V = r c_p \frac{\partial \theta}{\partial t} \]

\[ V = IR \]

\[ \vec{J} = -\sigma \nabla \phi \]
THE GOOD NEWS

• You don’t have to do this on your own...
• Software exists that solves these complex mathematical equations for you
THE BAD NEWS

- It is not a push button solution
- You need to have some understanding in order to get meaningful results fast...
How do FEM work?

The geometry is discretized into elements.

\[ y = f(x) \]

**UNKNOWN: \( y_1, y_2, \ldots, y_N \)**
How do FEM work? (cont.)

The underlying partial differential equation are written in an equivalent matrix form

$$\frac{\partial}{\partial x} \left(k \frac{\partial T(x)}{\partial x}\right) + Q_{ext} = 0 + \text{ BOUNDARY CONDITIONS}$$

$$= \begin{bmatrix}
    k_{11} & k_{12} & k_{13} & \cdots & k_{1n} \\
    k_{21} & k_{22} & k_{23} & \cdots & k_{2n} \\
    k_{31} & k_{32} & k_{33} & \cdots & k_{3n} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    k_{n1} & k_{n2} & k_{n3} & \cdots & k_{nn}
\end{bmatrix} \begin{bmatrix}
    T_1 \\
    T_2 \\
    \vdots \\
    T_n
\end{bmatrix} = \begin{bmatrix}
    b_1 \\
    b_2 \\
    \vdots \\
    b_n
\end{bmatrix}$$
What you need to do in preparation of a FEM analysis

• discretize the geometry
• define the initial conditions
• define the boundary conditions
• define the constitutive behavior of the material, e.g., for a thermal analysis you need:
  • select how fast the analysis will march in time (for a non-steady state analysis)
What the **FEM software** will do for you?

- convert the PDE to a system of algebraic equations (possibly non linear)
- (try to) solve the system of equations
- plot the results
What **you** need to do to successfully complete the analysis

- understand why the analysis fails (and it will...)
  (iterations divergence, severe element deformation, numerical instabilities)
- minimize the errors but selecting a adequately fine mesh
- validate convergence
- evaluate the importance and the effect of the various assumptions
A brief (and simple) example
Steady State Heat Transfer

\[ \frac{\partial}{\partial x} \left( \left( k\Theta + \frac{k l x}{L} \right) \left( \frac{d}{dx} \Theta(x) \right) \right) - 20 - 10x \]
We need to solve:

\[
100 \left( \frac{d}{dx} \theta(x) \right) + (1 + 100x) \left( \frac{d^2}{dx^2} \theta(x) \right) - 20 - 10x = 0
\]

\[
\theta(0) = 0 \quad \theta(L) = 100 \quad L = 1
\]

For this (very simple) case an analytical solution exists

\[
analytical\_sol := \frac{1}{40} x^2 + \frac{399}{2000} L
\]

\[
+ \frac{3}{200000} \ln(1 + 100x) \left( \frac{6651700 + 133 \ln(101)}{\ln(101)} \right) - \frac{399}{200000} \ln(1 + 100x)
\]
Discretization and basis functions

$h_i(x)$

$\theta_i h_i(x)$
Approximation of solution and boundary condition

\[ \theta(x) \approx \hat{\theta}(x) = \sum \theta_i h_i(x) \]
Residual

\[ 100 \left( \frac{d}{dx} \theta(x) \right) + (1 + 100x) \left( \frac{d^2}{dx^2} \theta(x) \right) - 20 - 10x = 0 \]

\[ \text{Residual}(x) = 100 \left( \frac{d\tilde{\theta}(x)}{dx} \right) + (1+100x) \left( \frac{d^2\tilde{\theta}(x)}{dx^2} \right) - 20 - 10\tilde{\theta}(x) \neq 0 \]
Minimization of Residual

\[ \text{Residual}(x) = f(\theta_1, \theta_2, \ldots, \theta_{N-1}, x) \]

\[ \text{CHOOSE } \theta_1, \theta_2, \ldots, \theta_{N-1} \]

\[ \text{TO MINIMIZE RESIDUAL} \]

(Galerkin, Least Square, Collocation)

\[ \text{LS} \rightarrow \min_{0}^{L} (\text{Residual}(x))^2 dx \]
N-2 equations (due to BC)

\[ EQ_1 = 4.078000001 \times 10^5 a_2 - 1.209500000 \times 10^5 a_3 - 300. - 4.577750000 \times 10^5 a_4 = 0 \]
\[ EQ_2 = -6.85700 \times 10^5 a_2 - 400.0000001 + 4.798000001 \times 10^5 a_3 - 1.189500000 \times 10^5 a_4 + 4.078000001 \times 10^5 a_1 = 0 \]
\[ EQ_3 = 4.798000001 \times 10^5 a_2 - 6.73700 \times 10^5 a_3 - 7.695400002 \times 10^6 + 3.918000001 \times 10^5 a_4 - 1.209500000 \times 10^5 a_1 = 0 \]
\[ EQ_4 = -1.189500000 \times 10^5 a_2 + 3.918000001 \times 10^5 a_3 - 1.0350250 \times 10^7 - 1.717250000 \times 10^5 a_4 = 0 \]

Solution := \{ a_1 = 37.12240624, a_2 = 70.18795206, a_3 = 96.14416984, a_4 = 110.4683584 \}
Analytical Solution

FEM solution
N=5

Residual

FEM solution
N=10

FEM solution
N=40
MACROSCOPIC FEM MODELING OF FAST
Sintering under electrical current is a strongly coupled problem.

Temperature dependence of resistivity

Joule heating

Effect of current on diffusion or plasticity

Density dependence of electrical properties

Thermal activation of sintering

Density dependence of thermal properties

Diffusion-based sintering

Electricity Transport

Thermal Analysis

Diffusion-based Sintering
Early modeling efforts

  - 1D, only compact and die, thermal only - not coupled with electric current
  - Steady state finite difference method of thermal/electric problem was dependent on material properties
Thermoelectric Coupling Models

• Zavaliangos, Zhang, Krammer, and Groza, Mater Sci Eng. 2004
  – Thermoelectrical coupling, recognized that the full system needs to be modeled, contact resistance
• Vanmeensel, Laptev, Hennicke, van der Biest Acta Met. 2005
  – Thermoelectric coupling, comparison with experiments for a conductor and an insulator
• Anselmi-Tamburini, Gennari, Garay and Munir, Mater. Sci. Eng. A 2005
  – Similar in Vanmeensel
• McWilliams B, Zavaliangos A, Cho KC, et al., JOM 2006
  – Role of part die dimensions on gradients
• Wang, Casolco, Xu and Garay, Acta Mat. 2007
  – Includes elastic stress from thermal expansion
“Simple” Thermoelectric FEM Analysis

- Thermal-Electrical coupled analysis
- No displacement degrees of freedom
- Material properties function of temperature
- Radiation to the chamber walls and between parts
- Conduction between parts is considered in the model
Temperature dependence of resistivity

Joule heating

Effect of current on diffusion or plasticity

Density dependence of electrical properties

Thermal activation of sintering

Density dependence of thermal properties
Modeling framework – theory

Conservation of charges

\[-\int_{V} \frac{d\phi}{dx} \cdot J dV = -\int_{S} \phi \cdot J \cdot n dS + \int \delta \phi \cdot n dS\]

Conservation of energy

\[\int_{V} \rho c_p \frac{\partial \theta}{\partial t} dV = \int_{V} \nabla (k \nabla \theta) dV + \int_{S} \dot{q}_c dV + \int_{S} (\dot{q}_{conv} + \dot{q}_r + \dot{q}_{ec}) dS\]

Temperature evolution
Heat conduction in component
Joule heating in component
Convection
Radiation
Heat conduction across surface
Joule heat at interface

Coupling (joule heating)

\[\dot{q}_e = E \cdot J = \frac{d\phi}{dx} \cdot (\sigma \frac{d\phi}{dx})\]

It does not look like it, but it is Ohm’s law
Constitutive equations

- Need to provide
  - Thermal properties
  - Electrical properties
- Can be temperature dependent
- Can be anisotropic (e.g., graphite sheets)
- Usually input in tabular form
Temperature dependent materials properties

**Graphite**

**Al₂O₃**

* Tokai G540 Data Sheet, Tokai Carbon Co. Ltd.
** Baikalox Ultra-Pure Alumina Data Sheet, Baikowski International Corporation.
Thermal & electric gap resistance

- A result of imperfect interfaces
- Electric gap resistance results in local heat at the interface
- Thermal gap resistance is effectively an insulator

Heat and current flux across the interface

\[
\dot{q}_c = h_g (\theta_1 - \theta_2)
\]

\[
J = \sigma_g (\varphi_1 - \varphi_2)
\]
Note that although the neck is an equipotential surface, the current density is not uniform—there is a peak at the root of the neck.

Holm’s resistance

$$R = \frac{\rho}{2a}$$
Holm’s contact resistance

\[ R_1 = \frac{\rho L}{A} \quad R_{Cj} = \frac{\rho}{2a_j} \]

\[ \frac{1}{R_C} = \sum \frac{2a}{\rho} \]
Contact resistance – size effect

For large scales, the behavior of contacts is relatively well known (Maxwell, Holm), the solution of the electrostatic problem provides an estimate of the contact resistance.

When the size of the contact ‘neck’ a decreases, the scattering length $L_s$ of the charges becomes comparable with the length scale of the contact – Knudsen effect

$$R = \frac{\rho}{2a} + \frac{4K}{3\pi a} \left( \frac{L_s}{a} \right)$$

Maxwell-Holm

Knudsen-Sharvin

The behavior becomes more complex at nanoscale
The presence of contamination on the surface of the powders usually means even higher contact resistance
Thermal and electric gap conductances

We group the contact resistances into two categories based on the orientation of interfaces: Horizontal contact conductances and vertical contact conductances.

Why different horizontal and vertical contact conductances?
Calibration of thermal & electric gap conductances

The gap conductances are determined by four independent calibration experiments and a series of numerical simulation runs.
Difference between (a) and (b)

- extra punch length (can be calculated) and
- extra contact resistance (can be extracted from the difference
  (careful that temperature gradient should be small)
Difference between (b) and (c)
  • presence of the die
  • presence of the vertical contact resistance
Difference between (b) and (c)

- vertical contact resistance is now over a smaller length
Flow chart

Run single punch and double punch experiments. Log potential, current and temperature.

Guess axial electric gap conductance and run single punch and double punch simulations and record potential, current and temperature.

No

Predicted resistance fits experimental single and double runs

Yes

Guess transverse electric gap conductance and use axial gap electric gap conductance from previous step. Run dummy test simulations. Record potential, current and temperature.

No

Predicted resistance fits experimental data of dummy run

Yes

Run experiment with graphite cylinder. Measure temperatures in the specimen and die surface simultaneously. Guess thermal gap conductance in transverse direction. Run simulation with graphite cylinder.

No

Predicted temperature difference fits experimental data of graphite cylinder runs

Yes

Derive thermal gap conductance in axial direction based on

\[
\sigma_g^h = 1.25 \times 10^7 (\Omega \cdot m^2)^{-1}; \]

\[
\sigma_g^v = 7.5 \times 10^6 (\Omega \cdot m^2)^{-1}; \]

\[
h_g^h = 2.2 \times 10^3 W/m^2\cdot K; \]

\[
h_g^v = 1.32 \times 10^3 W/m^2\cdot K \]

Typical values
Note proportionality
(assumes geometry effect only)
Close loop temperature control

A subroutine is developed to implement the control scheme. Simulation at preset heating profile can be realized.

\[ DU = -k (q_{\text{read}} - q_{\text{preset}}) \]
Dummy run calibration

No specimen
- Calibration experiment
Input = Temperature \( q(t) \)
Total system resistance decrease (top) and die surface temperature decreases as applied pressure increases as a result of the better contact. This affects local heat generation (at contacts) and heating loss along the axis.
Closing the parenthesis in contact resistance

- It is crucial as it affects current flow significantly.
- It is also crucial in terms of temperature distribution because contact resistances cause local heating.
- There are still issues because there is a complex dependence of thermal and electrical contact resistances on not just the material pair but — pressure, temperature (and time — creep).
- It is not straightforward to deal with this problem (especially in complex shapes).
Before pushing ahead with the FEM: A back of the envelope calculation
Simplified lumped electric circuit model

$R_{sys} = 0.5 \, \text{m}\Omega$ contains horizontal contact resistance

$R_p = 1.5 \, \text{m}\Omega$

$R_{sp} = \text{infinite for alumina powder and 0.3m}\Omega \text{ for graphite cylinder}$

$R_{die} = 0.5 \, \text{m}\Omega$

$$R = \frac{1}{\sigma A} \frac{L}{\pi}$$

$$R = \frac{1}{\sigma} \ln\left(\frac{R_{out}}{R_{in}}\right)$$
# Geometry, function and materials of each component

<table>
<thead>
<tr>
<th>Component</th>
<th>Resistance group</th>
<th>Function</th>
<th>Material</th>
<th>Outer Diam./ Inner Diam./ Thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$R_{sys}$</td>
<td>Water cooled Ram</td>
<td>Graphite</td>
<td>OD: 120, Th.: 200</td>
</tr>
<tr>
<td>B</td>
<td></td>
<td>Large disc, current transfer</td>
<td>Graphite</td>
<td>OD: 155, Th.: 20</td>
</tr>
<tr>
<td>C</td>
<td></td>
<td>Small disc, spacer</td>
<td>Graphite</td>
<td>OD: 120, Th.: 20</td>
</tr>
<tr>
<td>D</td>
<td></td>
<td>Spacer, thermal buffer</td>
<td>Graphite</td>
<td>OD: 76.2, Th.: 40</td>
</tr>
<tr>
<td>E</td>
<td>$R_p$</td>
<td>Punch</td>
<td>Graphite</td>
<td>OD: 19.1, Length: 25.4</td>
</tr>
<tr>
<td>F</td>
<td>$R_{die}$</td>
<td>Die</td>
<td>Graphite</td>
<td>OD: 44.6, ID: 19.1, Length: 38.1</td>
</tr>
<tr>
<td>G</td>
<td>$R_{sp}$</td>
<td>Specimen</td>
<td>Alumina, Graphite</td>
<td>OD: 19.1, Th.: 6.0</td>
</tr>
</tbody>
</table>
The amount of current flowing through specimen depends on the resistance ratio of specimen to die.

Maximum Joule heating in specimen when resistance is same as graphite die. Metallic powders may experience significant Joule heating during FAST, while ceramic powder will not.
Where does heating occur?

<table>
<thead>
<tr>
<th></th>
<th>System $R_{sys}$</th>
<th>Punch $R_p$</th>
<th>Die $R_{die}$</th>
<th>Specimen $R_{sp}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resistance, mΩ</td>
<td>1.0</td>
<td>3.0</td>
<td>0.5</td>
<td>0.3/infinite</td>
</tr>
<tr>
<td>Current</td>
<td>$I_0$</td>
<td>$I_0$</td>
<td>$\frac{R_{sp}}{R_{die} + R_{sp}} I_0$</td>
<td>$\frac{R_{die}}{R_{die} + R_{sp}} I_0$</td>
</tr>
<tr>
<td>Joule heat</td>
<td>$I_0^2 R_{sys}$</td>
<td>$I_0^2 R_P$</td>
<td>$\frac{(R_{sp})^2 R_{die}}{(R_{die} + R_{sp})^2} I_0^2$</td>
<td>$\frac{(R_{die})^2 R_{sp}}{(R_{die} + R_{sp})^2} I_0^2$</td>
</tr>
<tr>
<td>Joule heat %</td>
<td>0.24</td>
<td>0.71</td>
<td>0.03</td>
<td>0.03</td>
</tr>
<tr>
<td>(specimen: graphite)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Joule heat %</td>
<td>0.22</td>
<td>0.67</td>
<td>0.11</td>
<td>&lt;0.01</td>
</tr>
<tr>
<td>(specimen: alumina)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The maximum Joule heating is generated in the punches (~ 70%) independently of the resistivity of the specimen, mainly because the punches offer the smallest cross section.
Voltage drop across the specimen

The voltage drop across the specimen is only a small fraction of the total voltage difference applied on the system, $V_{tot}$.

The voltage across the specimen increases monotonically with $R_{sp}$. Its maximum value, $V_{sp}^{max}$, occurs when $R_{sp}$ approaches to infinity (insulating specimen):

$$V_{sp}^{max} = V_{tot} \frac{R_{die}}{R_{die} + R_p + R_{sys}}$$

This means that if the goal is to maximize the voltage across the specimen for an insulating specimen, the resistance of the die should be maximized ($R_{die} >> R_p + R_{sys}$).
Comparison of a conductive versus non-conductive sample

FEM model
Local potential difference is smaller than the overall one.

**Alumina:** Significant potential gradient exists across the specimen. About ~10% of the total $\Delta V$. The condition is often claimed to cause micro spark/plasma at particle contact – but the field is very small compared to what is needed for arcing/plasma etc.

**Graphite:** almost no potential gradient within sample. (~1-2% of the total $\Delta V$)

**CONDUCTIVE MATERIAL:** 
- Value: ~5V/m

**NON-CONDUCTIVE MATERIAL:** 
- Value: O[100 V/m]

Compare with values required for arcing (usually > 10,000V/m)
Notice the value of the current density

- Non-conductive material: ~Zero
- Conductive material: ~100 A/cm²
- Compare with values electromigration

Maximum at the end of punch end due to

Current is diverted towards the die due to the

...of total current goes through specimen
Joule heating is maximum at the end of punch end due to smallest cross section area in the system. Joule heating is almost zero for both alumina and graphite cylinder. 

Alumina: because all current passes through die. 

Graphite: because of low resistivity of specimen.
Joule heating in specimen

Joule heating is maximum with graphite specimen. The observation is consistent with lumped resistance model.

Joule heating in specimen is small (<1%) compared with punches. In terms of specimen heating, heat conduction is more important than Joule heating.
Validation study
Temperature evolution

Generated heat is partially diffused into the specimen and partially conducted into the machine and radiated from die surface.

The pattern of heat flow results in temperature of specimen is higher than the control temperature on the surface of the die by at least 100°C.

Highest temperature develops in the punches during the early stages.
Evolution of temperature on the surface of the die – comparison of prediction and experiment. A and B represent two instances, just after the beginning of heating and at the late heating stage, respectively.
Evolution of resistance of the system

With the incorporation of contact resistance, the calculated resistance of system matches experimental data in both cases.

The difference in FAST of Al₂O₃ at initial stage is caused by (1) presence of nano particles at interface between punch and die during filling, and (2) inaccuracy of electric conductivity of graphite at lower temperature (<300°C).
Temperature difference

- Experimental data shows the temperature excess of interior temperatures $\theta_{\text{center}}$ over the die surface temperature $\theta_{\text{surface}}$.

- The incorporation of thermal contact resistance enables the simulated results to match experimental data.

- To know the true specimen temperature, a calibration-based correction with respect to surface temperature is necessary.
The actual heating rate is linearly proportional to the heating rate on the die surface and it is higher than the die surface temperature of 70%. The linear relation between the heating rate in the specimen and on the die surface indicates that a single calibration for the specific die/punch configuration suffices to cover a large range of heating rate.
Overestimation of the thermal diffusivity. For a 50% lower thermal diffusivity the corresponding temperature difference increases by about 80%. (doubtful)

Underestimation of the emissivity of the die surface. Using emissivity of $\varepsilon=1.0$ instead of the value $\varepsilon=0.8$ results in a 10% increase of the temperature difference. (insignificant)

The presence of thermal contact resistance on the inner vertical surface of the die. By scaling the contact resistance it is possible to match exactly the experimental data. (most probable explanation)
At low temperature heat conduction through the loading train is dominant.

Radiation becomes more important at higher temperatures.

FAST of high melting point materials requires radiation shielding.
Energy efficiency

The total energy input into the system (normalized by $mC_p\Delta T$, temperature ramp from 25 °C to 1100 °C) as a function of electric gap conductance.

There is a transition of energy efficiency in the range of electric gap conductance of $10^4(Wm^2)^{-1}$. Above this level, the conversion of electric energy is not efficient.
The effect of punch length

- Gradient to die surface not affected
- The main difference is the maximum transient temperature in the punch that can reach locally
- For the predicted values the punches may deform by creep

McWilliams B, Zavaliangos A, Cho KC, et al., JOM 2006
Effect of die diameter on sample center to die surface gradient

Smaller die reduces the temperature difference between the specimen center and the die surface

→ Important design consideration for process control
→ Tradeoff between mechanical strength and gradient
Summery of early FEM results

- A coupled thermal-electric-densification with temperature close-loop controlling finite element analysis has been implemented.

- A detailed evaluation of the accuracy of the model has been conducted for electrically conductive and insulator materials. The evaluation, compared with experimental measurement, indicates that the model provides a reasonably accurate prediction of thermal and electric response.

- Specimen is mainly heated up by heat conduction from punch irrespective of its resistivity. The most critical location for such temperatures is in the punches – high resistance (low cross section area=high Joule heating).

- These temperatures may reach 200-600°C above the specimen temperature – graphite may creep. Longer punches are particularly prone to this problem.
Some more results: 3D case study

- Gradients become more complex when processing complex shapes and/or larger specimens
- Simulation as a design tool becomes critical

![Graph showing temperature distribution with a note of ~150°C difference of compact edges!]
3D simulations

• Can we reduce the gradients in the sample in a “complex” shaped part to get uniform temperature distribution?

• One possibility: Electrically insulate punches to control current flow through sample

Current can only pass through red areas
Temperature distribution in compact
How to insulate?

• Punch inserts → material possibilities?
  – Zirconia: Tm=2700°C, ρ=10^{11} Ohm*m k=1.15 W/mK
  – BN: Tm=3000°C, ρ=7e-5 Ohm*m, k=20 W/mK
• External heating of die
  – Thermally insulate sample
Potential issues & Ideas

• Current now only passes through parts of sample rather than the entire volume
  – If there is an effect of current it will be seen here as temperature is (roughly) the same but the current is different
SINTERING + THERMOELECTRIC MODEL

• McWilliams & Zavaliangos, J. Mat. Sci. 2008
  – Coupled sintering and thermoelectric
Motivation

Complex shapes that evolve substantial during sintering

Simple thermoelectrical model does not suffice

Also the simple stepwise approximation of sintering in a thermoelectrical model works for cylindrical sample but not for complex shape
Prior work was mainly on the thermal+electrical problem but...

With the introduction of a sintering model the way opens for full coupling (i.e. for incorporation of current effects on diffusion or plasticity)
Introduction of a sintering model (e.g., Bouvard et al)

\[
\begin{align*}
\tilde{\varepsilon}^{\text{tot}} &= \frac{-P + \sigma_s}{3K} \tilde{I} + \frac{1}{2G} \sigma' + \tilde{\varepsilon}^{\text{rev}} \\
\dot{\varepsilon}^{\text{tot}} &= \dot{\varepsilon}^{s} + \dot{\varepsilon}^{\text{vp}} + \dot{\varepsilon}^{\text{rev}} = \mathbf{\dot{\varepsilon}}_{ij}
\end{align*}
\]

\(\tilde{\varepsilon}^{s}\) = sintering strain rate

\(\tilde{\varepsilon}^{\text{vp}}\) = viscoplastic strain rate

Experiments to fit expression

\[
\dot{\varepsilon}_{s} = \Omega(T)(\rho_{\infty}(T) - \rho)^n
\]

IMPLEMENTED IN USER CREEP SUBROUTINE IN ABAQUS

Creep subroutine details

ABAQUS estimates elastic and viscoplastic strains

Prescribed BCs and loads \( \sigma_t, dt \)

Subroutine solves for strain increment based on constitutive eqns.

\[ \Delta \varepsilon^{cr} \]

\[ \dot{\varepsilon}_s = \Omega(T)(\rho_\infty(T) - \rho)^n \]

\( \Omega, \rho, \) and \( n \) evaluated at \( T_t \)

Equilibrium

Updated density
Coupling algorithm schematic

- **RD₀**
  - **t₀, θ₀** → **t₁, θ₁**
    - Thermal-electric simulation
    - θ(t)
    - Properties function of local density
    - Temperature evolves
    - Mesh does not evolve

- **RD₁**
  - **t₀, θ₀** → **t₁, θ₁** → **t₂, θ₂**
    - Sintering simulation
    - Updated mesh
    - Thermal-electric simulation
    - θ(t)
    - Thermal history from TH-EL step
    - Mesh evolves due to sintering
Solution requires convergence study

Typically 50-100 steps within the range of densification are more than adequate
Testing the algorithm

• 2D case study
  – Rectangular compact
  – Free sintering (no applied load)
    (load can be done but interaction with dies requires delicate handling in this simulation)

• Purpose
  – Verify sintering algorithm
  – Confirm that the evolution of density plays a role
  – Evaluate effect of initial density distributions and material properties on overall sintering kinetics under coupled thermal-electric conditions

McWilliams & Zavaliangos, J. Mat. Sci. 2008
“Paper” Study

• 2 RD₀ configurations of conductive material
  – 80% low / 20% high density material arranged in series
  – 80% low / 20% high density material arranged in parallel

• Repeat with thermal diffusivity (α) reduced by order of magnitude

• NO DIE, TO VISUALIZE RESULTS
IN A DIE THERE WOULD BE INTERNAL STRESSES
TDE model - Density evolution

**SERIES**

**High alpha**

**Low alpha**

**PARALLEL**

**High alpha**

**Low alpha**
High thermal conductivity
Two layers in series

- Most of the Joule heating $I^2R$ occurs in the low density layer due to higher resistivity.
- Thermal diffusivity is high enough to homogenize the temperature, minimal intermediate distortion.
Low thermal conductivity
Two layers in series

- Joule heating $I^2R$ in the low density layer create temperature gradient
- Strong intermediate distortion as low density layer densifies first!
High thermal conductivity
Two layers in parallel

- Most of the Joule heating $V^2/R$ occurs in the high density layer (!)
- Minimal intermediate distortion because thermal diffusivity is high enough to homogenize the temperature
Low thermal conductivity
Two layers in parallel

- Most of the Joule heating $V^2/R$ occurs in the high density layer.
- Strong intermediate distortion as high density layer densifies first!
Low thermal conductivity
Series vs Parallel at intermediate time

- Note that strong intermediate distortion has opposite curvatures
Message

Understanding the interplay between current, temperature & sintering can help us optimize complex sintering operations under electrical current.
COMPLEX SHAPE
FAST
SYSTEM + COMPACT
SINTERING + THERMOELECTRICAL
SIMULATION
Application of fully coupled model to complex shape sintering

- New
  - **Applied load**
  - Uniform initial RD<sub>0</sub>
  - More complex heat transfer
    - Contact with punches and die
    - Conduction to/from heat sources/sinks
  - Axisymmetric

- Thermal electric part:
  - Conduction, convection, and radiation
  - Stepwise current profile

Top and bottom T fixed at 15°C
Fully coupled (TDE) vs thermoelectric (TE)

$\Delta T$ from sample center to die surface (cylindrical geometry)

$TDE = \text{thermal} + \text{sintering} + \text{electrical}$

$TE = \text{thermal} + \text{electrical}$
Material in center of compact heats up first due to heat from punches and heat loss to die → this material begins to densify first and leads to a situation similar to parallel configuration of previous case study

Fully dense material properties used for TE simulation
Explanation

Temperature gradient

Densification gradient

Current gradient (current prefers to go through the more densified area)

Pressure gradient (more densified area supports higher stress)

Even if at the end of the day the density is similar (tends to 100%) different parts of the sample will undergo different temperature/densification history
ELECTRIC CURRENT DENSITY THROUGH THE SPECIMEN INCREASES DUE TO DENSIFICATION

![Graph showing the evolution of electric current density](image)

Figure 4.6 Evolution of electric current density (ECD, A/m²) distributions within the punch/die/compact assembly for the thermal-electric-sintering model with cylindrical specimen (half model shown).
relative density and temperature

$t=645s$

$t=676s$

$t=840s$

Half models
Applied stress = 2.8 MPa
Effect of load on sintering (cylinder)

The graph shows the relative density over time for two different loads: 2.8 MPa (blue line) and 4.2 MPa (pink line). The x-axis represents time in seconds, ranging from 400 to 1100, and the y-axis represents relative density, ranging from 0 to 1.2. The graph illustrates the sintering process at different loads, with a notable increase in relative density between 700 and 800 seconds.
A “fully” coupled model has been implemented in FEM

• Predictions are as good as the data we put in 😊
• A “good” sintering model is needed
• If there is coupling of current and sintering then a sintering model with E effects should be implemented (no additional computational difficulty)
The big challenge

• Coupling of sintering and electrical effects
  Although the presented work provides the framework for FEM modeling of FAST the key problem appears to be delineating the coupling of sintering and current
MICROSCOPIC CONSIDERATIONS

Some (not so) random thoughts
DOES SIZE MATTER?

If the same contact go through these two arrangements of particles which contacts see higher current density?

\[ \frac{d_1}{\alpha_1} = \frac{d_2}{\alpha_2} \]
THE TWO ARRANGEMENTS SEE THE SAME CURRENT DENSITY 😃

THE CURRENT DENSITY IS AMPLIFIED AT THE NECK BY $(d/\alpha)^2$
Contact resistance – size effect

For large scales, the behavior of contacts is relatively well known (Maxwell, Holm), the solution of the electrostatic problem provides an estimate of the contact resistance.

When the size of the contact ‘neck’ \( a \) decreases, the scattering length \( L \) of the charges becomes comparable with the length scale of the contact – Knudsen effect

\[
R = \frac{\rho}{2a} + \frac{4K}{3\pi a} \left( \frac{L}{a} \right)
\]

Maxwell-Holm \hspace{1cm} Knudsen-Sharvin

Still this does not imply that the current density on nanoscale contacts will be much higher.
Note that although the neck is an equipotential surface
The current density is not uniform – there is a peak at the root of the neck
At low densities

the local current density

is x2-3 times higher
due to the isolated paths

**Electric current density**

**REMEMBER THE VALUE OF CURRENT DENSITY?**

Conductive material: 
\[ \sim 100 \text{ A/cm}^2 \]

multiplied by \( (d/\alpha)^2 \) or more

\[ \sim 10000 \text{ A/cm}^2 \] for small neck

This is electromigration maybe even electroplasticity territory

**HOWEVER THIS AMPLIFICATION IS SIGNIFICANT ONLY AT THE VERY EARLY STAGE OF DENSIFICATIONS**
Electroplasticity (?)

Fig. 9. Effect on the tensile flow stress of MgO at 1600°C upon application ('on') and removal ('off') of a d.c. electric field $E = 220$ V cm$^{-1}$. From Conrad and Yang [14].

Conrad MSE A322 (2002) 100–107
Electromigration

Fig. 8.20. Concentration profile of Sb after electromigration in copper at 866°C (Cu–0.8 wt.% Sb alloy between the weld planes SE, copper on the outside). After Th. Hehenkamp, Göttingen.
Power input patterns

Same power input: \( V^2 t = \text{const.} \)

F: Fourier number
Temperature evolution: DC vs. pulse current

Top: DC

Right: Double-pulse
Temperature evolution: DC vs. pulse

Viewports:
- DC: Single pulse
- Double-pulse: Two pulses
Temperature distribution

Pulse current offers more uniform temperature distribution than DC at the end of heating.
Is the contact much hotter than the bulk of the powder particle?

For a 10 micron typical conductive ($\lambda=1\times10^{-5} \text{ m}^2/\text{s}$) powder
A temperature difference between the contact and the center will homogenize within $5-10 \times R^2/\lambda = 12.5-25 \mu\text{s}$

Almost instantaneous homogenization of temperature differences.

Unless the powder particle is very large (>100 micron) the temperature between contact and particle bulk is almost the same...
Food for thought

• Experimental determination/delineation of current vs non-current effects
• Proper model calibration
• Models for small size (non-continuum)
• Understanding of local chemistry
WHAT MODELING IS NOT

WHAT INDUSTRY WANTS

WHAT ACADEMIA OFFERS
MODELING IS A TOOL

1980s  1990s  2000s