Modelling and FEM simulation of electric field assisted sintering of tungsten carbide (WC)

Sree Koundinya
s.sistla@iwm.rwth-aachen.de

Follow this and additional works at: http://dc.engconfintl.org/efa_sintering

Part of the Engineering Commons

Recommended Citation
Modelling and FEM Simulation of Electric Field Assisted Sintering of Tungsten Carbide (WC)

S.K.Sistla, M.Hajeck, A.Kaletsch, C.Broeckmann

Institute for Materials Applications of Mechanical Engineering

Electric Field Assisted Sintering and Related Phenomena Far from Equilibrium, ECI Conference, Tomar(Portugal), 11.03.2016
Previous Work

Cylindrical Sample

Bi Layer Laminate Sample

[C. van Nguyen, S.K. Sistla et.al Japanese Ceramic Society 2016]
Outline

- Introduction
  - Motivation
  - Objectives
  - Research Hypothesis

- Modelling Field Assisted Sintering (FAST)
  - Modeling densification
  - Material parameters

- Results
  - SPS Experiments with WC
  - Coupled structural thermal electrical simulation

- Conclusion

- Outlook
**Introduction**

**Motivation**
- FAST is an emerging powder consolidation technique
- Limited numerical investigations of FAST
- Complex material transport mechanisms

**Objectives**
- Model the densification behavior from existing FAST models.
- Model inelastic strain components for building a material model
- Correlate the experimental behavior with the numerical simulations

**Research Hypothesis**
- Selection of a conducting material (here binder less WC)
- SPS Experiments to determine the boundary conditions
- Build coupled structural thermal electrical simulations
- Verify the simulation results such as densification
Outline

- Introduction
  - Motivation
  - Objectives
  - Research Hypothesis

- Modelling Field Assisted Sintering (FAST)
  - Modeling densification
  - Material parameters

- Results
  - SPS Experiments with WC
  - Coupled structural thermal electrical simulation

- Conclusion

- Outlook
Modelling Field Assisted Sintering

- Modelling densification

\[ \varepsilon_{ij} = \varepsilon_{ij}^{el} + \varepsilon_{ij}^{inel} \]
\[ \Delta \varepsilon_{ij}^{inel} = \Delta \varepsilon_{ij}^{cr} + \Delta \varepsilon_{ij}^{sw} \]

Constitutive Model for FAST of Conductive Materials [1]

\[ \dot{\varepsilon} = \dot{\varepsilon}_{gb} + \dot{\varepsilon}_{cr} \]

Total Strain rate due to grain boundary diffusion

\[ \dot{\varepsilon}_{gb} = \dot{\varepsilon}_{gb}^{em} + \dot{\varepsilon}_{gb}^{st} + \dot{\varepsilon}_{gb}^{dl} \]

Strain rate component due to electro migration

\[ \dot{\varepsilon}_{gb}^{em} = - \frac{\delta_{gb} D_{gb}}{kT} \left( \frac{Z^* e_q}{(2r+r_p)^2} \right) \frac{U}{l} \]

Strain rate component due to sintering stress

\[ \dot{\varepsilon}_{gb}^{st} = - \frac{\delta_{gb} D_{gb}}{kT} \frac{\Omega}{(2r+r_p)^2} \left\{ \frac{3\alpha}{2r} \left[ \frac{1}{r_p} - \frac{1}{4r} \right] \right\} \]

Strain rate component due to external load

\[ \dot{\varepsilon}_{gb}^{dl} = \frac{\delta_{gb} D_{gb}}{kT} \frac{\Omega}{(2r+r_p)} \left\{ \frac{\sigma_Z}{4r^2} \right\} \]

[1-Olevsky 2006]
Modelling Field Assisted Sintering

- Modelling densification

Based on the continuum theory of sintering [2]

\[ \sigma_z = A_1 W^{m-1} \left[ \varphi \dot{\varepsilon}_{crz} + \left( \psi - \frac{1}{3} \varphi \right) (\dot{\varepsilon}_{cr} + \dot{\varepsilon}_{crz}) \right] + \sigma_s \]  

8

Since, WC is a single phase material \( m = 1 \) and from boundary conditions \( \dot{\varepsilon}_{cr} = 0 \)

Total Strain rate due to Power law creep \( \dot{\varepsilon}_{crz} = \frac{\dot{\sigma}_z + \frac{\sigma_{kk}}{3} - \sigma_s}{A_1(\psi + \frac{2}{3} \varphi)} \)  

9

\[ \varphi = \rho^2, \quad \psi = \frac{2}{3} \frac{\rho^3}{(1-\rho)}, \quad \sigma_s = \frac{3 \alpha}{2r} \rho^2 \]  

10

With conservation of mass

\[ \dot{\rho} = -\rho \dot{\varepsilon}_{kk} \]  

11

[2-Olevsky 1998]
Modelling Field Assisted Sintering

- Material parameters

<table>
<thead>
<tr>
<th>Material</th>
<th>Material Property</th>
<th>Value</th>
<th>Literature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tungsten Carbide (WC)</td>
<td>Density</td>
<td>15250 kg/m³</td>
<td>[3]</td>
</tr>
<tr>
<td></td>
<td>E-Modulus</td>
<td>600 GPa</td>
<td>[3]</td>
</tr>
<tr>
<td></td>
<td>Poisson's Ratio</td>
<td>0.3</td>
<td>[3]</td>
</tr>
<tr>
<td></td>
<td>Thermal Conductivity</td>
<td>28 W/m.K</td>
<td>[3]</td>
</tr>
<tr>
<td></td>
<td>Specific Heat</td>
<td>292 J/kg.K</td>
<td>[3]</td>
</tr>
<tr>
<td></td>
<td>Electrical Conductivity</td>
<td>2.39 S/m</td>
<td>[3]</td>
</tr>
<tr>
<td>Graphite</td>
<td>Density</td>
<td>1850 kg/m³</td>
<td>[4]</td>
</tr>
<tr>
<td></td>
<td>E-Modulus</td>
<td>200 GPa</td>
<td>[4]</td>
</tr>
<tr>
<td></td>
<td>Poisson's Ratio</td>
<td>0.3</td>
<td>[4]</td>
</tr>
<tr>
<td></td>
<td>Thermal Conductivity</td>
<td>65-1.7x10⁻²T W/m.K</td>
<td>[4]</td>
</tr>
<tr>
<td></td>
<td>Specific Heat</td>
<td>310.5+1.7xT J/kg.K</td>
<td>[4]</td>
</tr>
<tr>
<td></td>
<td>Electrical Conductivity</td>
<td>1/(26-3x10²T+2x10⁻⁵T²-6.4x10⁻⁹T³ +7.8x10⁻¹³T⁴) x10⁶ S/m</td>
<td>[4]</td>
</tr>
</tbody>
</table>

[4-Song 2011]
### Modelling Field Assisted Sintering

- Model parameters

<table>
<thead>
<tr>
<th>Material</th>
<th>Material Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tungsten Carbide (WC)</td>
<td>Initial Relative Density</td>
<td>0.8259</td>
</tr>
<tr>
<td></td>
<td>Initial grain size</td>
<td>30 µm</td>
</tr>
<tr>
<td></td>
<td>Equivalent Charge</td>
<td>1.9226e-18 C</td>
</tr>
<tr>
<td></td>
<td>Atomic Volume</td>
<td>1.294e-29 m³</td>
</tr>
<tr>
<td></td>
<td>Surface Tension</td>
<td>1.12 J/m²</td>
</tr>
<tr>
<td></td>
<td>Grain-boundary diffusion frequency factor</td>
<td>50e-10m³/s</td>
</tr>
<tr>
<td></td>
<td>Activation energy for grain-boundary diffusion</td>
<td>309616 J/mol</td>
</tr>
<tr>
<td></td>
<td>Activation energy for power-law creep</td>
<td>591000 J/mol</td>
</tr>
<tr>
<td></td>
<td>Power-law creep frequency factor</td>
<td>261 MPa/s</td>
</tr>
<tr>
<td></td>
<td>Electrical Field per Unit length</td>
<td>900 V/m</td>
</tr>
</tbody>
</table>
Modelling Field Assisted Sintering

- Implementation of densification model

Densification Model
( User Subroutine CREEP )

Part Geometry
( ABAQUS CAE )

Coupled Structural Thermal Electrical Model

ABAQUS Standard

Initial Conditions – Temperature, Interactions

Boundary Conditions – Voltage, Pressure

Post Processing
( ABAQUS ODB )

Relative density, Volumetric Changes, Stresses, etc.
Outline

Introduction
- Motivation
- Objectives
- Research Hypothesis

Modelling Field Assisted Sintering (FAST)
- Modeling densification
- Material parameters

Results
- SPS Experiments with WC
- Coupled structural thermal electrical simulation

Conclusion

Outlook
Results

- SPS Experiments at 1900°C
- Heating Rate 200 K/min
- Holding Time 2 min

Results as input for FEM Simulations

Results for verification of FEM Simulations
Results

- SPS Experiments at 2000°C
- Heating Rate 200 K/min
- Holding Time 2 min

Results as input for FEM Simulations

Results for verification of FEM Simulations
Results

Symmetric Model
Results

- SPS Experiments at 1900°C
- Heating Rate 200 K/min
- Holding Time 2 min

Results as input for FEM Simulations

Results for verification of FEM Simulations
Results

- SPS Experiments at 1900°C
- Heating Rate 200 K/min
- Holding Time 2 min

Relative Density Evolution
Results

- SPS Experiments at 2000°C
- Heating Rate 200 K/min
- Holding Time 2 min

Results as input for FEM Simulations

Results for verification of FEM Simulations
Results

- Sensitivity Analysis SPS Experiments at 1900°C
Results

- Sensitivity Analysis SPS Experiments at 2000°C
Outline

- Introduction
  - Motivation
  - Objectives
  - Research Hypothesis

- Modelling Field Assisted Sintering (FAST)
  - Modeling densification
  - Material parameters

- Results
  - SPS Experiments with WC
  - Coupled structural thermal electrical simulation

- Conclusion

- Outlook
Conclusion

- Mass transport mechanisms for FAST can be investigated and analyzed with coupled structural, thermal and electrical FEM simulations in a single step.

- Electrical field influences densification for conducting materials.

- Coupled electrical thermal simulations gives an insight into accurate prediction of the temperature gradient in the powder and computational time is shorter.
Outline

- Introduction
  - Motivation
  - Objectives
  - Research Hypothesis

- Modelling Field Assisted Sintering (FAST)
  - Modeling densification
  - Material parameters

- Results
  - SPS Experiments with WC
  - Coupled structural thermal electrical simulation

- Conclusion

- Outlook
Outlook

- Material properties for the powder and the tools dependent on relative density and temperature need to be experimentally determined for more accurate FAST simulations.

- Further numerical investigations need to be carried out to reduce the non-convergence caused due to nonlinearity in material modelling and contacts (thermal, mechanical and structural).

- Model parameters need to be accurately estimated for effective estimation of densification and volumetric changes.

- With more experiments and material characterization a better understanding and modifications would be proposed to the existing constitutive equation for densification by FAST.
We appreciate the help of Global Tungsten & Powders for supply of WC powder!

Thank you for your kind attention!

Sree Koundinya Sistla

IWM – Institute for Materials Applications in Mechanical Engineering
RWTH Aachen University
Augustinerbach 4
52062 Aachen

www.iwm.rwth-aachen.de