Winter 3-11-2016

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

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

Recommended Citation

[1] M. Abouaf, J. Chenot, G. Raisson and P. Bauduin, "Finite element simulation of Hot isostatic pressing of metal powders," International Journal of Numerical Methods Engineering, Vol.25, pp. 191-212, 1988. [2] H. Riedel and B. Blug, "A comprehensive model for solid state sintering and its application to silicon carbide," in Multiscale Deformation and Fracture in Materials and Structures, Springer Netherlands, pp. 49-70,2002. [3] T. Kraft and H. Riedel, "Numerical simulation of solid state sintering; model and application," Journal of the European Ceramic Society, vol. 24, no. 2, pp. 345-361, 2004. [4] Z. Shen, M. Johnsson, Z. Zhao and M. Nygren, "Spark Plasma Sintering of Alumina.," Journal of the American Ceramic Society, no. 85, p. 1921–1927, 2002. [5] Y. Song, Y. Li, Z. Zhau, Y. Lai and Y. Ye, "A multi-field coupled FEM model for one-step-forming process of spark plasma sintering considering local densification of powder material," Journal of materials science, vol. 46, no. 17, pp. 5645-5656, 2011.

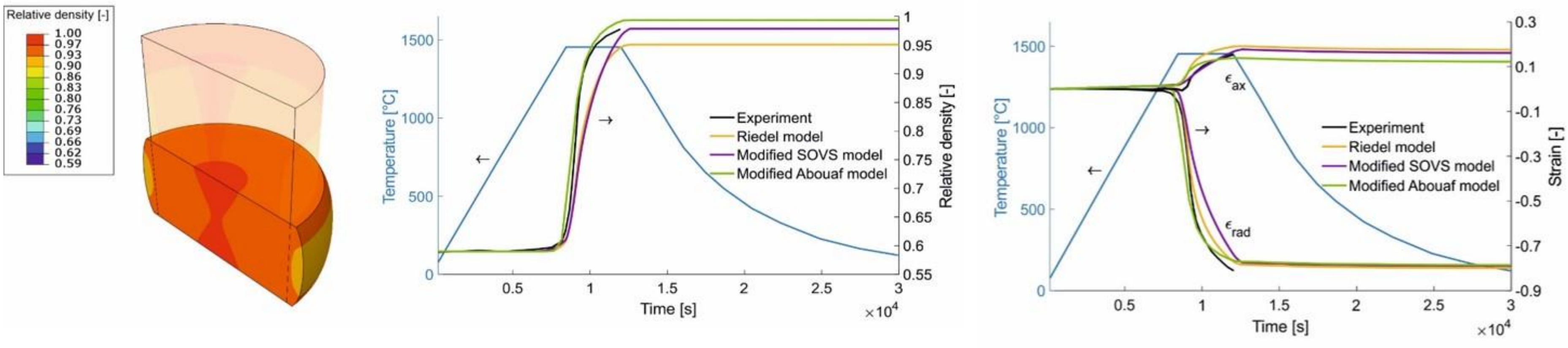
Modelling and FEM Simulation of Electric Field Assisted Sintering of Tungsten Carbide (WC)

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

$$\varepsilon_{ij} = \varepsilon_{ij}^{el} + \varepsilon_{ij}^{inel}$$ 1

$$\Delta\varepsilon_{ij}^{inel} = \Delta\varepsilon_{ij}^{cr} + \Delta\varepsilon_{ij}^{sw}$$ 2

Constitutive Model for FAST of Conductive Materials [1]

$$\dot{\varepsilon} = \dot{\varepsilon}_{gb} + \dot{\varepsilon}_{cr}$$ 3

Total Strain rate due to grain boundary diffusion $\dot{\varepsilon}_{gb} = \dot{\varepsilon}_{gb}^{em} + \dot{\varepsilon}_{gb}^{st} + \dot{\varepsilon}_{gb}^{dl}$ 4

Strain rate component due to electro migration $\dot{\varepsilon}_{gb}^{em} = -\frac{\delta_{gb} D_{gb}}{kT} \frac{Z^* e_q}{(2r+r_p)^2} \frac{U}{l}$ 5

Strain rate component due to sintering stress $\dot{\varepsilon}_{gb}^{st} = -\frac{\delta_{gb} D_{gb}}{kT} \frac{\Omega}{(2r+r_p)^2} * \left\{\frac{3\alpha}{2r}\left[\frac{1}{r_p} - \frac{1}{4r}\right]\right\}$ 6

Strain rate component due to external load $\dot{\varepsilon}_{gb}^{dl} = \frac{\delta_{gb} D_{gb}}{kT} \frac{\Omega}{(2r+r_p)} * \left\{\frac{\overline{\sigma_z}}{4r^2}\right\}$ 7

[1-Olevsky 2006]

Modelling Field Assisted Sintering

- Modelling densification

Based on the continuum theory of sintering [2]

$$\sigma_z = A_1 W^{m-1}\left[\varphi\dot{\varepsilon}_{crz} + \left(\psi - \frac{1}{3}\varphi\right)(\dot{\varepsilon}_{crr} + \dot{\varepsilon}_{crz})\right] + \sigma_s \quad 8$$

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

Total Strain rate due to Power law creep $\dot{\varepsilon}_{crz} = \frac{\acute{\sigma}_z + \frac{\sigma_{kk}}{3} - \sigma_s}{A_1\left(\psi + \frac{2}{3}\varphi\right)}$ 9

$$\varphi = \rho^2,\ \psi = \frac{2}{3}\frac{\rho^3}{(1-\rho)},\ \sigma_s = \frac{3\alpha}{2r}\rho^2 \quad 10$$

With conservation of mass

$$\dot{\rho} = -\rho\dot{\varepsilon}_{kk} \quad 11$$

[2-Olevsky 1998]

Modelling Field Assisted Sintering

- Material parameters

Material	Material Property	Value	Literature
Tungsten Carbide (WC)	Density	15250 kg/m^3	[3]
	E-Modulus	600 GPa	[3]
	Poisson's Ratio	0.3	[3]
	Thermal Conductivity	28 W/m.K	[3]
	Specific Heat	292 J/kg.K	[3]
	Electrical Conductivity	2.39 S/m	[3]
Graphite	Density	1850 kg/m^3	[4]
	E-Modulus	200 GPa	[4]
	Poisson's Ratio	0.3	[4]
	Thermal Conductivity	$65-1.7x10^{-2}T$ W/m.K	[4]
	Specific Heat	310.5+1.7xT J/kg.K	[4]
	Electrical Conductivity	$1/(26-3x10^{2}T+2x10-^{5}T^{2}-6.4x10^{-9}T^{3}+7.8x10^{-13}T^{4})x10^{6}$ S/m	[4]

[3-http://www.azom.com/properties.aspx?ArticleID=1203]
[4-Song 2011]

Modelling Field Assisted Sintering

- Model parameters

Material	Material Property	Value
Tungsten Carbide (WC)	Initial Relative Density	0.8259
	Initial grain size	30 µm
	Equivalent Charge	1.9226e-18 C
	Atomic Volume	1.294e-29 m^3
	Surface Tension	1.12 J/m^2
	Grain-boundary diffusion frequency factor	50e-10m^3/s
	Activation energy for grain-boundary diffusion	309616 J/mol
	Activation energy for power-law creep	591000 J/mol
	Power-law creep frequency factor	261 MPa/s
	Electrical Field per Unit length	900 V/m

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)

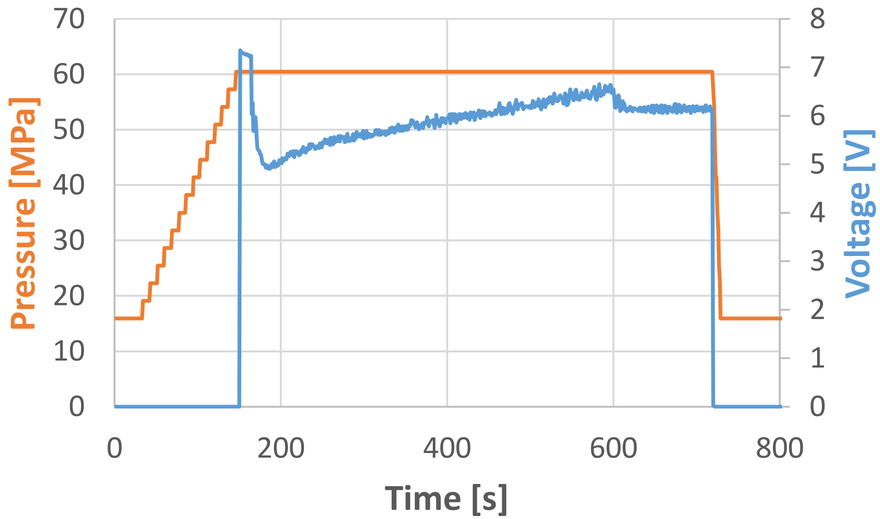
Relative density, Volumetric Changes, Stresses, etc.

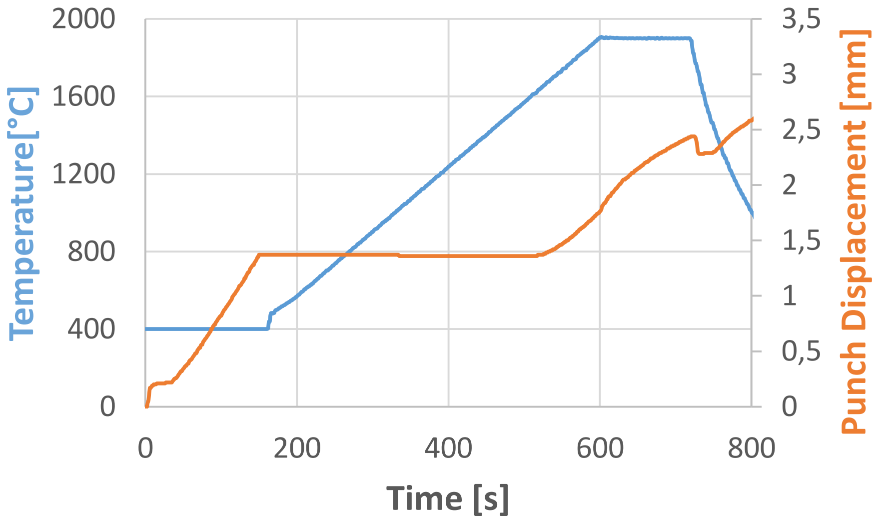
Outline

- **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



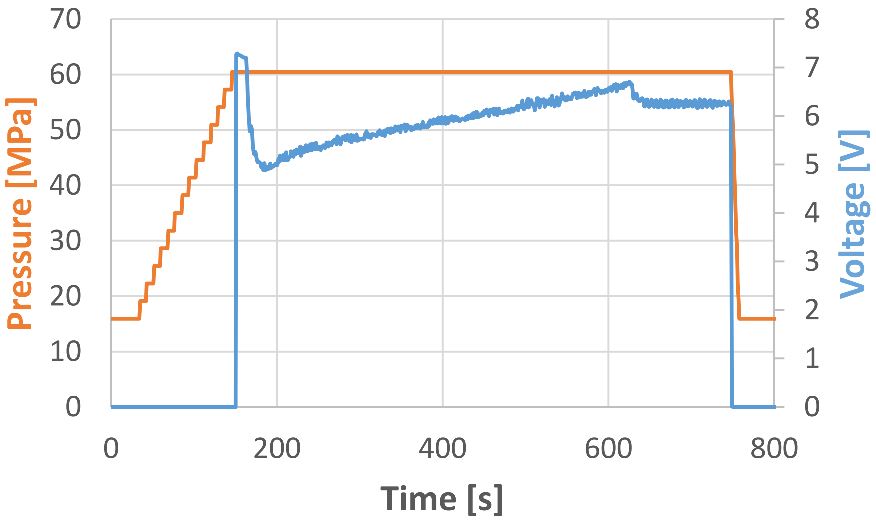


Results as input for FEM Simulations

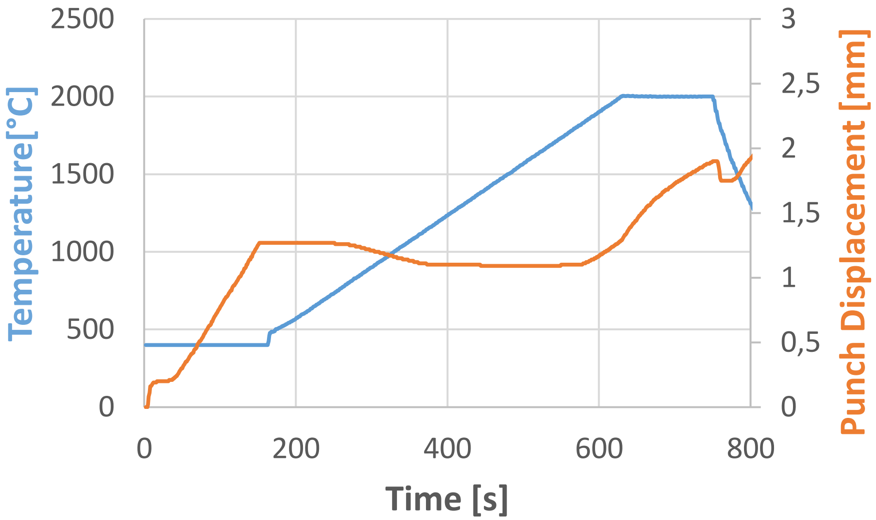
Results for verification of FEM Simulations

Results

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

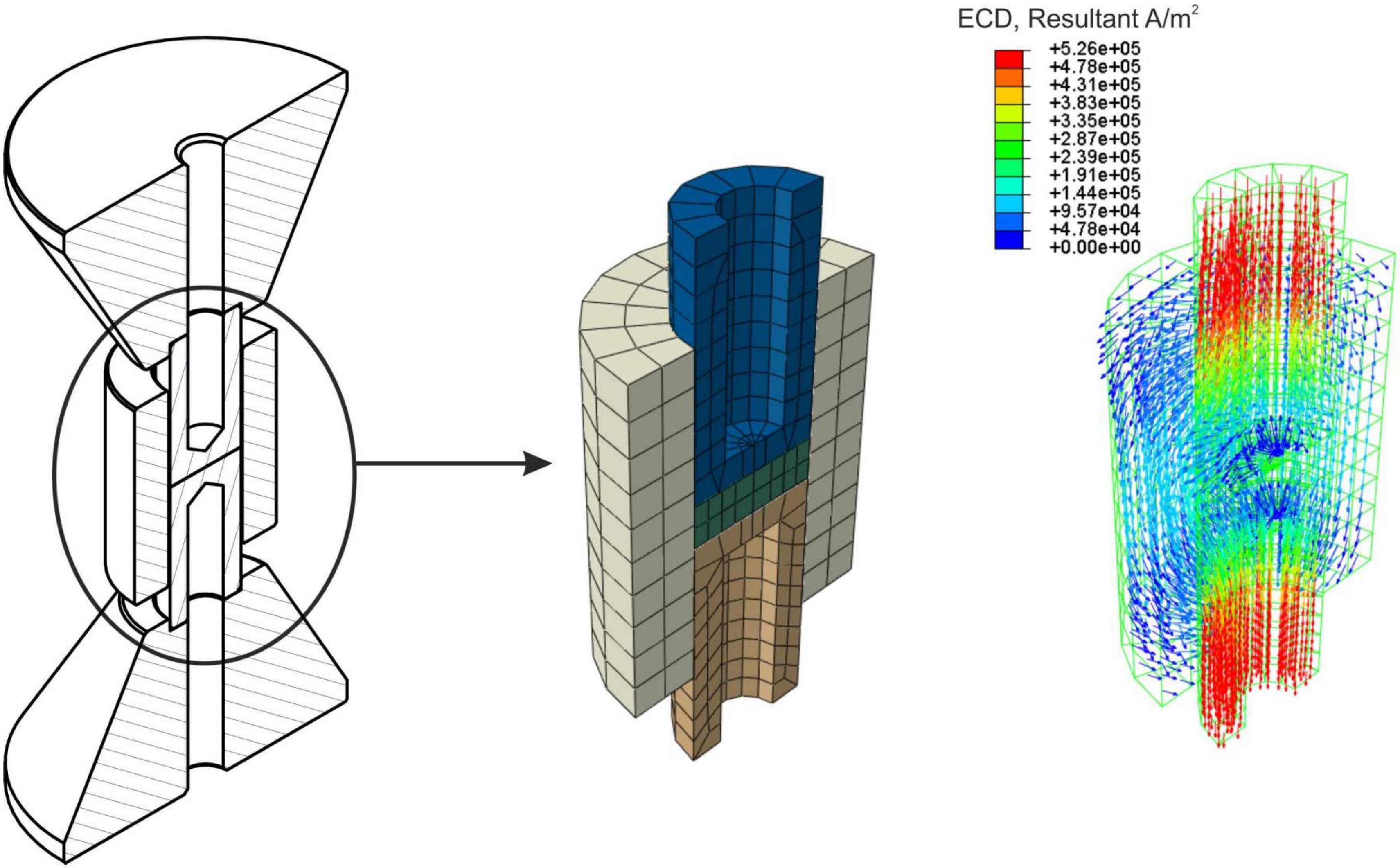


Results as input for FEM Simulations



Results for verification of FEM Simulations

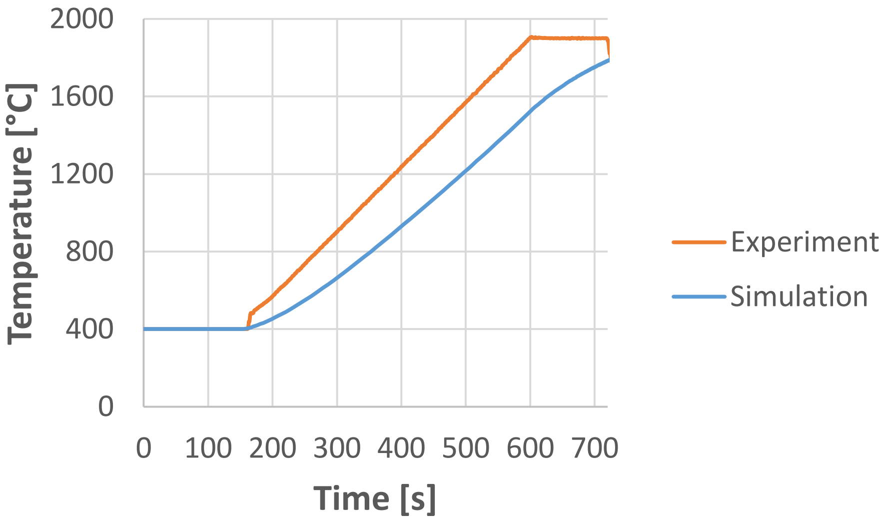
Results

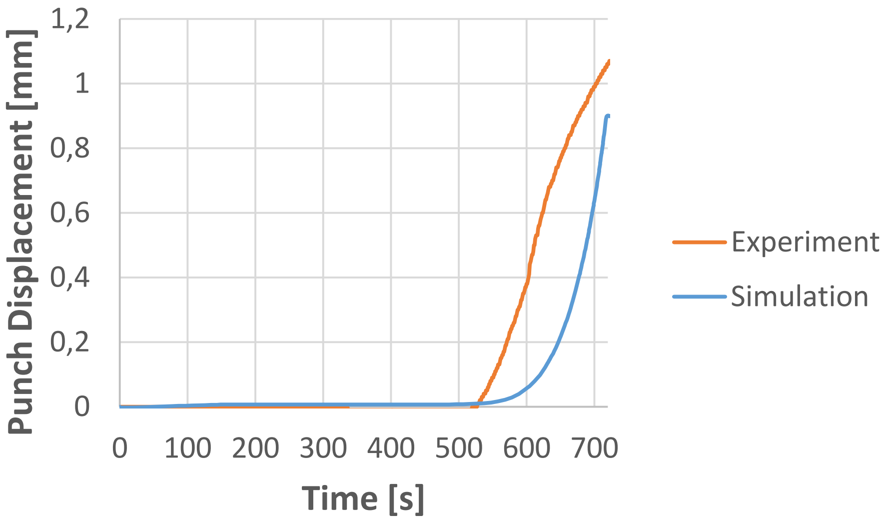


Symmetric Model

Results

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



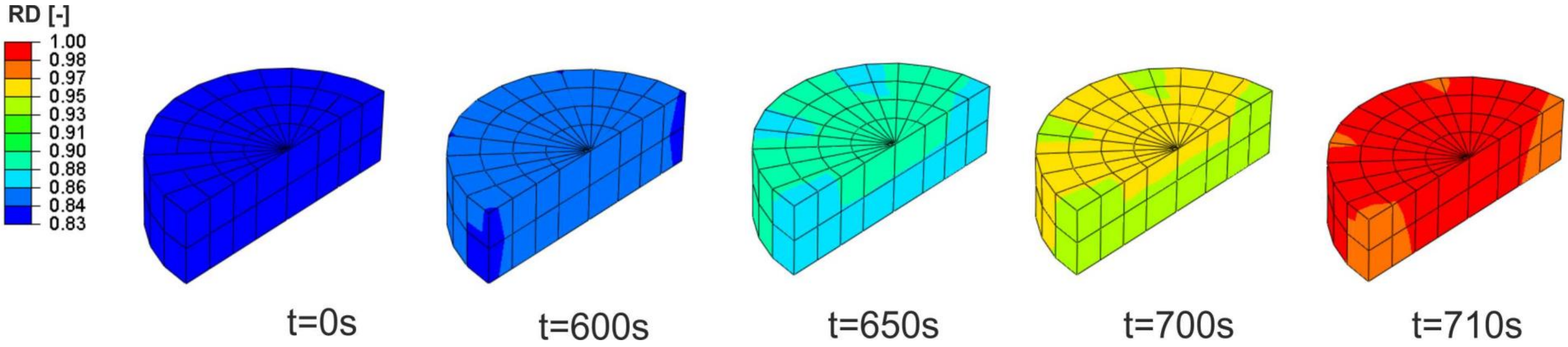


Results as input for FEM Simulations

Results for verification of FEM Simulations

Results

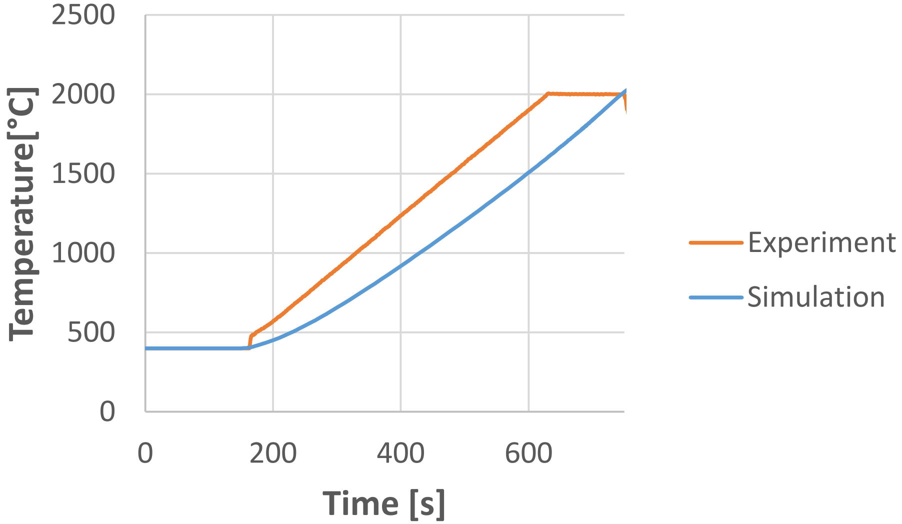
- SPS Experiments at 1900°C
- Heating Rate 200 K/min
- Holding Time 2 min

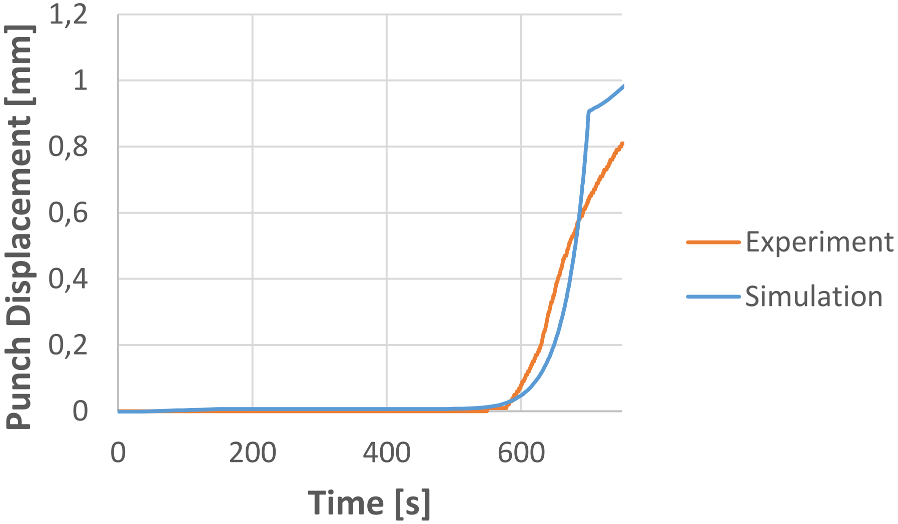


Relative Density Evolution

Results

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



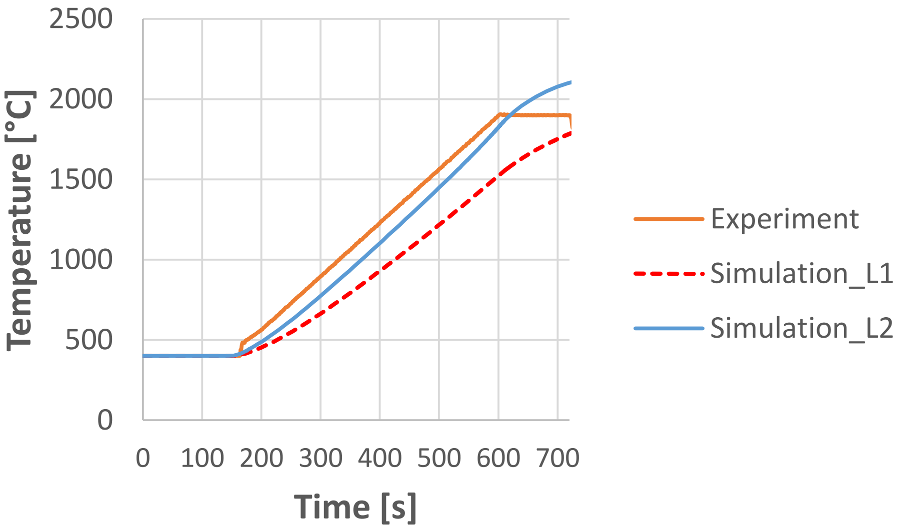


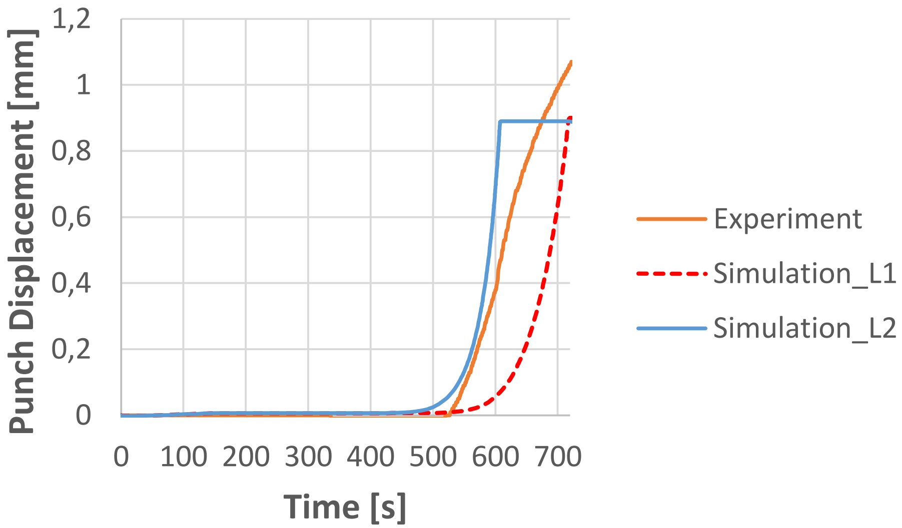
Results as input for FEM Simulations

Results for verification of FEM Simulations

Results

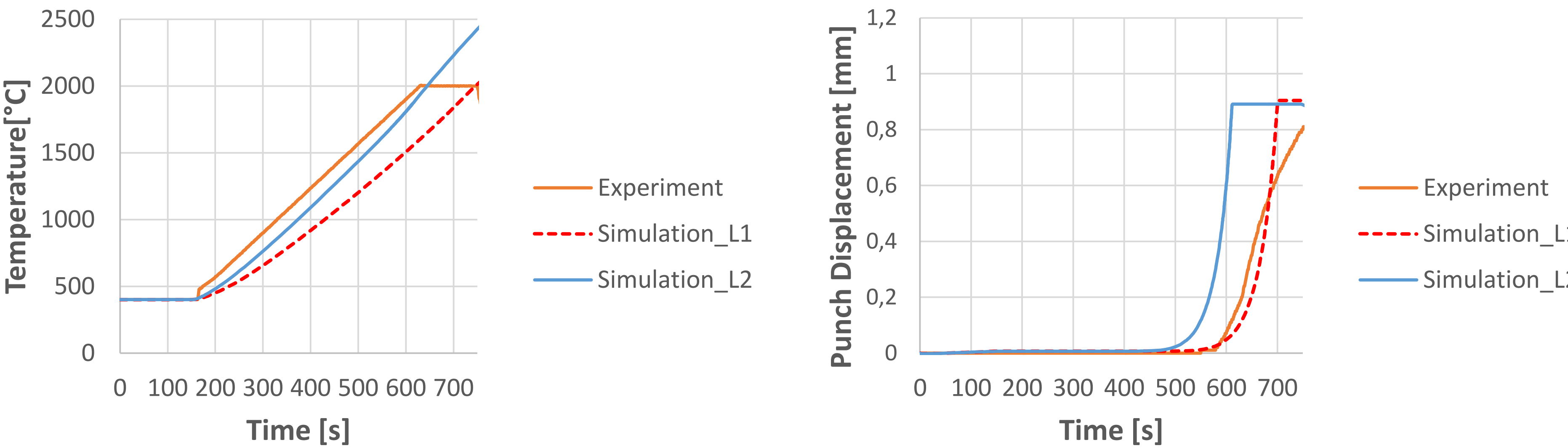
- Sensitivity Analysis SPS Experiments at 1900°C





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