

Microscopic Simulation of Solid State Sintering Regarding Irregularly Shaped Powder Particles

Max Weiner

July 28, 2023

Contents

Preface	4
1 Introduction	5
1.1 The RefraBund Project	5
1.1.1 Aim and Scope	5
1.1.2 Project Structure	5
1.1.3 Process Routes	5
1.2 State of the Art	5
1.2.1 Basic Theory of Sintering	5
1.2.2 Sintering Models with Sharp Interfaces	5
1.2.3 Sintering Models with Diffuse Interfaces	5
1.2.4 Monte-Carlo-Methods (MCM)	5
1.2.5 The Thermodynamic Extremal Principle (TEP)	5
1.2.6 Miscellaneous	6
2 Aim and Scope	7
3 Powder Analysis and Representation	8
3.1 Classic Methods of Powder Characterization	8
3.2 Particle Description by Parametrized Shape Functions	8
3.3 Characterization of Powders and Powder Mixtures	8
4 Model Development	9
4.1 A Discrete Model of Powder Particles	9
4.2 Considerations on Free Surfaces	9
4.3 Considerations on Grain Boundaries	9
4.4 Considerations on Sinter Necks	9
4.5 Considerations on Grain-Matrix Interfaces	9
4.6 Application of the Thermodynamic Extremal Principle (TEP)	9
5 Software Implementation of the Model	10
5.1 Representation of Particles and Nodes	10
5.2 Numerical Solution Procedure	10
5.3 Calculation and Extraction of Key Features	10
6 Model Validation	11
6.1 Investigations on Simple Test Cases	11
6.1.1 A Single Particle Free in Space	11
6.1.2 A Particle Pair Free in Space	11
6.1.3 A Particle Pair at Different Contact Angles	11
6.1.4 A Particle Pair with Asymmetric Material Properties	11
6.1.5 A Single Particle Embedded in a Matrix	11

6.1.6	A Particle Pair Embedded in a Matrix	11
6.2	Experimental Validation Counter Bulk Sintering Trials	11
7	Summary and Outlook	12
	List of Figures	13
	List of Tables	14

Preface

1 Introduction

1.1 The RefraBund Project

1.1.1 Aim and Scope

1.1.2 Project Structure

1.1.3 Process Routes

1.2 State of the Art

1.2.1 Basic Theory of Sintering

1.2.2 Sintering Models with Sharp Interfaces

1.2.3 Sintering Models with Diffuse Interfaces

1.2.4 Monte-Carlo-Methods (MCM)

Classic Monte Carlo Methods

Kinetic Monte Carlo Methods

1.2.5 The Thermodynamic Extremal Principle (TEP)

Classic Formulation

$$\mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) = \frac{\partial G(\mathbf{X}, \mathbf{x})}{\partial \mathbf{x}} \cdot \dot{\mathbf{x}} \rightarrow \max_{\dot{\mathbf{x}}} \quad (1.1a)$$

$$\mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) - \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) = 0 \quad (1.1b)$$

$$\mathcal{L} = \mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) + \lambda (\mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) - \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}})) \quad (1.2)$$

$$\mathcal{L}_{\dot{\mathbf{x}}} = (1 + \lambda) \frac{\partial G(\mathbf{X}, \mathbf{x})}{\partial \mathbf{x}} - \lambda \frac{\partial \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}})}{\partial \dot{\mathbf{x}}} \quad (1.3a)$$

$$\mathcal{L}_\lambda = \mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) - \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) \quad (1.3b)$$

Generalized Formulation

Acc. to Hackl2020

$$\mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) = \frac{\partial G(\mathbf{X}, \mathbf{x})}{\partial \mathbf{x}} \cdot \dot{\mathbf{x}} \rightarrow \max_{\dot{\mathbf{x}}} \quad (1.4a)$$

$$\mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) - \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) = 0 \quad (1.4b)$$

$$\mathbf{f}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j}) = 0 \quad (1.4c)$$

$$\mathbf{g}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j}) = 0 \quad (1.4d)$$

$$\mathcal{L} = \mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) + \lambda_1 (\mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) - \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}})) + \boldsymbol{\lambda}_2 \cdot \mathbf{f}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j}) + \boldsymbol{\lambda}_3 \cdot \mathbf{g}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j}) \quad (1.5)$$

$$\mathcal{L}_{\dot{\mathbf{x}}} = (1 + \lambda_1) \frac{\partial G(\mathbf{X}, \mathbf{x})}{\partial \mathbf{x}} - \lambda_1 \frac{\partial \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}})}{\partial \dot{\mathbf{x}}} + \boldsymbol{\lambda}_2 \frac{\partial \mathbf{f}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j})}{\partial \dot{\mathbf{x}}} + \boldsymbol{\lambda}_3 \frac{\partial \mathbf{g}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j})}{\partial \dot{\mathbf{x}}} \quad (1.6a)$$

$$\mathcal{L}_{\lambda_1} = \mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) - \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) \quad (1.6b)$$

$$\mathcal{L}_{\lambda_2} = \mathbf{f}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j}) \quad (1.6c)$$

$$\mathcal{L}_{\lambda_3} = \mathbf{g}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j}) \quad (1.6d)$$

1.2.6 Miscellaneous

2 Aim and Scope

3 Powder Analysis and Representation

3.1 Classic Methods of Powder Characterization

3.2 Particle Description by Parametrized Shape Functions

3.3 Characterization of Powders and Powder Mixtures

4 Model Development

4.1 A Discrete Model of Powder Particles

- Particles, Coordinate System
- Node Types
- Multi-Scale Considerations, Matrix

4.2 Considerations on Free Surfaces

4.3 Considerations on Grain Boundaries

4.4 Considerations on Sinter Necks

4.5 Considerations on Grain-Matrix Interfaces

4.6 Application of the Thermodynamic Extremal Principle (TEP)

5 Software Implementation of the Model

Reference to open source code

5.1 Representation of Particles and Nodes

- Classes
- Tree Structure
- Coordinate Systems

5.2 Numerical Solution Procedure

- TEP Solution
- Time Step
- Monte-Carlo Drawing

5.3 Calculation and Extraction of Key Features

- Volume Cell, Shrinkage
- Neck Measures

6 Model Validation

6.1 Investigations on Simple Test Cases

- 6.1.1 A Single Particle Free in Space**
- 6.1.2 A Particle Pair Free in Space**
- 6.1.3 A Particle Pair at Different Contact Angles**
- 6.1.4 A Particle Pair with Asymmetric Material Properties**
- 6.1.5 A Single Particle Embedded in a Matrix**
- 6.1.6 A Particle Pair Embedded in a Matrix**

6.2 Experimental Validation Counter Bulk Sintering Trials

7 Summary and Outlook

List of Figures

List of Tables