

Microscopic Simulation of Solid State Sintering Regarding Irregularly Shaped Powder Particles

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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

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

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

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

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

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

Generalized Formulation

Acc. to Hackl2020

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

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

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

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

$$\mathcal{L} = \mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) + \lambda_1 (\mathcal{D}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}) - \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}})) + \lambda_2 \cdot \mathbf{f}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j}) + \lambda_3 \cdot \mathbf{g}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j}) \quad (1.5)$$

$$\mathcal{L}_{\dot{\mathbf{x}}} = (1 + \lambda_1) \frac{\partial G(\mathbf{X}, \mathbf{x})}{\partial \mathbf{x}} - \lambda_1 \frac{\partial \mathcal{Q}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}})}{\partial \dot{\mathbf{x}}} + \lambda_2 \frac{\partial \mathbf{f}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j})}{\partial \dot{\mathbf{x}}} + \lambda_3 \frac{\partial \mathbf{g}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{j})}{\partial \dot{\mathbf{x}}} \quad (1.6a)$$

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

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

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

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

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