Microscopic Simulation of Solid State Sintering Regarding Irregularly Shaped Powder Particles

Max Weiner

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General things about internal state and non-equilibrium

Classic Formulation

The classic formulation of the principle was basically formulated by Svoboda and Turek [3], however dependent on the works of Ziegler [4, 5] and Onsager [2].

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

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

$$\mathcal{L} = \mathcal{D}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) + \lambda \left(\mathcal{D}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) - \mathcal{Q}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) \right) \tag{1.2}$$

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

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

Generalized Formulation

Acc. to Hackl, Fischer, and Svoboda [1]

$$\mathcal{D}(\boldsymbol{X}, \boldsymbol{x}, \dot{\boldsymbol{x}}) = \frac{\partial G(\boldsymbol{X}, \boldsymbol{x})}{\partial \boldsymbol{x}} \cdot \dot{\boldsymbol{x}} \to \max_{\dot{\boldsymbol{x}}} \tag{1.4a}$$

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

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

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

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

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

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

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

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

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6.1.6 A Particle Pair Embedded in a Matrix

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Bibliography

[1] Klaus Hackl, Franz Dieter Fischer, and Jiri Svoboda. "Constraints in Thermodynamic Extremal Principles for Non-Local Dissipative Processes". In: *Continuum Mechanics and Thermodynamics* 32.5 (Sept. 2020), pp. 1337–1345. ISSN: 0935-1175, 1432-0959. DOI: 10.1007/s00161-019-00846-3. URL: http://link.springer.com/10.1007/s00161-019-00846-3 (visited on 08/12/2022).

[2] Lars Onsager. "Reciprocal Relations in Irreversible Processes. I." In: *Physical Review* 37.4 (Feb. 15, 1931), pp. 405–426. ISSN: 0031-899X. DOI: 10.1103/PhysRev.37.405. URL: https://link.aps.org/doi/10.1103/PhysRev.37.405 (visited on 07/18/2023).

[3] J. Svoboda and I. Turek. "On Diffusion-Controlled Evolution of Closed Solid-State Thermodynamic Systems at Constant Temperature and Pressure". In: *Philosophical Magazine B* 64.6 (Dec. 1991), pp. 749–759. ISSN: 1364-2812, 1463-6417. DOI: 10.1080/13642819108207635. URL: https://www.tandfonline.com/doi/full/10.1080/13642819108207635 (visited on 08/11/2022).

[4] H. Ziegler. *An Introduction to Thermomechanics*. New York: North Holland Publishing, 1983.

[5] H. Ziegler. "Some Extremum Principles in Irreversible Thermodynamics, with Application to Continuum Mechanics". In: *Progress in Solid Mechanics* 4 (1963), p. 91.