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Sintering Process Simulation of a Solid Oxide Fuel Cell Anode and Its Predicted Thermophysical Properties

Pei Fu ¹, Min Yan ², Min Zeng ¹ and Qiuwang Wang ^{1,*}

1 Key Laboratory of Thermo-Fluid Science and Engineering, MOE, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi, 710049, P.R. China

2 School of Energy Engineering, Western Mine Exploitation and Hazard Prevention of the Ministry of Education, Xi'an University of Science & Technology, Xi'an, Shaanxi, 710054, P.R. China

*Corresponding author: Tel and Fax: +86(29)82665539; E-mail: wangqw@mail.xjtu.edu.cn

Highlights

1. A CG-MD method is improved to simulate the sintering process of SOFC anode.
2. Nanostructure and relevant thermal properties of the sintered anode are obtained.
3. Effects of sintering conditions and composition are systematically investigated.
4. Analyses and predictions provide a guide to obtain the desired properties.

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