

Supplementary Materials for

W–CeO₂ Core–Shell Powders and Macroscopic Migration of the Shell via Viscous Flow during the Initial Sintering Stage

Haitao Yang^{1,2,†}, Ningfei Zhang^{1,†}, Chan Wang³ and Qingyu Hou^{1,*}

¹ School of Metallurgical Engineering, Anhui University of Technology, Maanshan 243032, China; ngyanghaitao@163.com.cn (H.Y.); zhangningfei@ahut.edu.cn (N.Z.)

² Nanjing Iron and Steel Co., Ltd., Nanjing 210035, China

³ Deyang Sanhuan Technology Co., Ltd., Deyang 618000, China; 18855576276@163.com

* Correspondence: qingyuhou@hotmail.com or houqingyu@ahut.edu.cn; Tel./Fax: +86-555-2311570

† These authors contributed equally to this work.

$$\sum_{i=A,B,C} \phi_i = 1 \quad S(1)$$

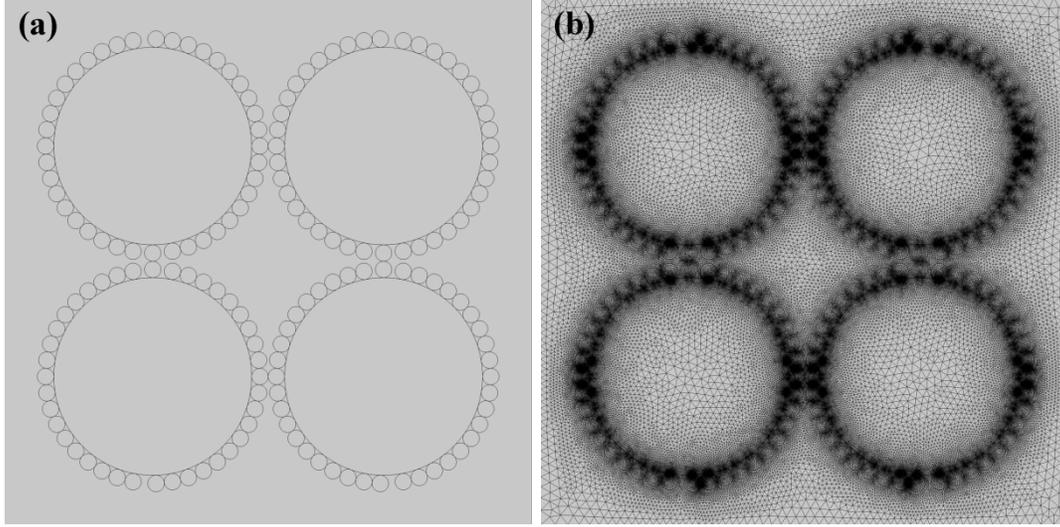


Figure S1. Schematic of the four-ball model composed of core-shell W-CeO₂ structure (a) and (b) the unstructured triangular mesh with interfacial refinement (the small balls and the big balls represent respectively CeO₂ and W, and the others represent 10⁻³ Pa vacuum).

$$\sum_i |\nabla\phi_i|^2 = \sigma_{ij} + \sigma_{ik} - \sigma_{jk} \quad S(2)$$

where i, j and k were respectively phase A, B, and C; σ_{ij} , σ_{ik} , and σ_{jk} were respectively the surface tensions between phase A and phase B, phase A and phase C, phase B and phase C.

$$F = \int \left[\frac{12}{\varepsilon} f(\phi_A, \phi_B, \phi_C) + \frac{3}{8} \varepsilon \sum_A |\nabla\phi_A|^2 + \frac{3}{8} \varepsilon \sum_B |\nabla\phi_B|^2 + \frac{3}{8} \varepsilon \sum_C |\nabla\phi_C|^2 \right] \quad S(3)$$

where $f(\phi_A, \phi_B, \phi_C)$ was bulk free energy density function; $\frac{3}{8} \varepsilon \sum_i |\nabla\phi_i|^2$ ($i=A, B$, and C , interface gradient free energy) was capillary term, which was a function or parameter specifying the additional free bulk energy ($\sum_i |\nabla\phi_i|^2$, capillary coefficient); ε was the parameter controlling interface thickness, which could be chosen larger than its theoretical value without modifying the capillary properties of the interfaces from a numerical point of view ^[1].

$$f(\phi_A, \phi_B, \phi_C) = \sigma_{AB} \phi_A^2 \phi_B^2 + \sigma_{AC} \phi_A^2 \phi_C^2 + \sigma_{BC} \phi_B^2 \phi_C^2 + \phi_A \phi_B \phi_C (\sum_A |\nabla\phi_A| + \sum_B |\nabla\phi_B| + \sum_C |\nabla\phi_C|) \quad S(4)$$

$$\frac{\partial\phi_i}{\partial t} = \nabla \cdot \left(\frac{M_0}{\sum_i} \nabla\eta_i \right) \quad S(5)$$

where t was the time; M_0 was the chemical mobility related to phase field variables, which was the parameter determine the time scale of the Cahn–Hilliard diffusion and it thereby also governed the diffusion-related time scale for the interface; η_i could be expressed by Eq. S(6) [1].

$$\eta_i = \frac{4\Sigma_T}{\varepsilon} \sum_{j \neq i} \left(\frac{1}{\Sigma_j} \left(\partial_i f(\Phi_A, \Phi_B, \Phi_C) - \partial_j f(\Phi_A, \Phi_B, \Phi_C) \right) \right) - \frac{3}{4} \varepsilon \Sigma_i \nabla^2 \Phi_i \quad S(6)$$

where $i, j \in (A, B, C)$; Σ_T was defined in Eq. S(7) [1].

$$\frac{3}{\Sigma_T} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C} \quad S(7)$$

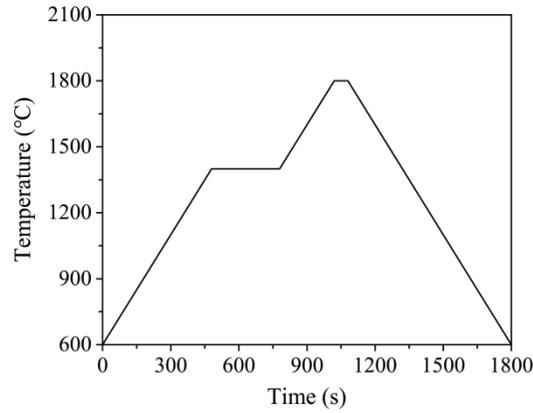


Figure S2. The interpolation function $int(t)$ used for FEM simulation.

$$\vec{\mathbf{n}}_{\text{wall}} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0 \quad S(8)$$

$$\vec{\mathbf{n}}_{\text{wall}} \cdot \frac{3}{4} \varepsilon \Sigma_i \nabla \Phi_i = \frac{3}{4} \varepsilon \Sigma_i |\nabla \Phi_i| \cos(\theta_i) \quad S(9)$$

[1] Boyer F, Lapuerta C, Minjeaud S, et al. Cahn–Hilliard/Navier–Stokes model for the simulation of three-phase flows[J]. *Transport in Porous Media*, 2010, 82: 463-483.