Meso-Scale Phase-Field Modeling of Microstructural Evolution in Solid Oxide Fuel Cells

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Microstructural evolution occurs in solid oxide fuel cells (SOFCs) during operation, which cause severe electrochemical performance degradation as well as structural failure such as crack formation. Nickel (Ni) particle coarsening is believed to cause microstructural evolution in the Ni-based anode of SOFCs. Furthermore, the accumulation of expanded pores during the microstructural evolution is responsible for crack formation. Based on the diffuse-interface theory and the phase-field method, integrating both Cahn-Hilliard equation and Ginzburg-Landau equation, a meso-scale phase-field model was established to investigate microstructural evolution and crack formation in the Ni / Yttria Stabilized Zirconia (YSZ) anode of SOFCs. Then, the model was applied to explore the coupling effects of microstructural evolution on SOFCs performance degradation. Simulation results show that particle size, porosity, and particle size ratio of Ni-YSZ are most influential parameters in microstructural evolution. It was found that the triple phase boundaries (TPBs) area was decreased by 24% and power density was decreased by 11.03% after 1000 hours of operation. In addition, the power density was decreased by 27%. This work is expected to provide us a comprehensive understanding of SOFCs' microstructural evolution as well as a tool for SOFC's performance degradation analysis.

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Solid oxide fuel cells (SOFCs) could be one possible solution to the depleting energy resources of the modern world due to its fuel flexibility, low carbon emissions, and high efficiency. With up to 60% energy efficiency and a life expectancy of 40,000 hours, the SOFC has emerged as an ideal candidate to meet the energy challenges of the modern world.1–3 However, the commercialization of SOFC is hindered due to its high operating temperature, manufacturing cost, and structural instability.4,5 Structural evolution of SOFC often leads to the structural failure and shortening of SOFC lifetime.6,7 Moreover, structural evolution results in compromising SOFCs’ electrochemical performance, mostly in the electrodes.

A SOFC consists of both electrodes (i.e., anode and cathode) and a ceramic electrolyte. The anode is consisted of ion conducting phase and electron conducting phase to facilitate the fuel oxidation reaction.2 The cathode reduces the oxygen into oxygen ion, which is then diffused to anode through the ceramic electrolyte, such as yttria stabilized zirconia (YSZ).10 Electrochemical reaction of SOFC mainly occurs in the triple phase boundary (TPB) area,1,11 where the pore phase, the ion conducting phase, and electron conducting phase join to convert chemical energy of fuel gases to electrical energy.1,6,11 TPB area is the key microstructural property controlling the electrochemical activities of SOFC.14 It is desired to have a stable microstructure with optimized TPB area.15,16 However, recent studies reveal that TPB area is often diminished due to microstructure evolution.10,17–20 The microstructure evolution is controlled by the Ni particle coarsening, which in turn leads to the performance degradation and crack formation. Particle coarsening process was first reported by Ostwald et al.21 In detail, Ostwald ripening refers to the late stage of phase separation. The phase-field method separates an immiscible binary mixture into a domain pure in each component. It applies different orientation fields to defining the crystallographic orientations of experimentally observed phenomena such as evaluating SOFCs’ performance in the long term. In this modeling work, the coarsening of Ni particle is considered as a capillarity driven phenomena.20 According to the Gibbs-Thomson effect, materials with high curvature regions have higher chemical potential than that of the lower curvature regions, this difference in chemical potential controls the transporta-

The total free energy function is governed by the dominant transport mechanism (i.e., surface- and volume-diffusion) of Ni particle.11 Additionally, high operating temperature of SOFC leads to the enhanced mass transport of Ni particle.12 During its operation, the surface diffusivity (or mobility) of Ni particle is much higher than that of the YSZ particle, which essentially makes YSZ stationary or non-evolving compared to the Ni particle,13–28 serving as the supporting structure in which Ni coarsens and evolves via diffusion along Ni-pore interfaces. Moreover, the evolution of the microstructure leads to the pore size growth and the accumulation of expanded pores during the surface- and volume-diffusion, which causes crack formation.26 However, it is quite challenging capturing microstructural evolution due to explicit tracking of the interface moving boundaries.

To overcome the aforementioned issue, researchers have been applying the phase-field method for investigating the variety of interfacial phenomena among different immiscible interfaces, microstructural evolution, and crack formation.13,28 The phase-field method, which allows explicit tracking of the phase interfaces, has emerged as a powerful computational method for modeling transport phenomena and complex microstructural evolution process.29 In addition, the modeling approach allows visualizing the microstructural evolution in two- and three-dimensional.30 The phase-field method separates an immiscible binary mixture into a domain pure in each component. It applies different orientation fields to defining the crystallographic orientations of

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Ni- and YSZ phases. The interfacial dynamics of the anode is defined by a variable called Order Parameter (OP) (i.e., phase-field variable). For instance, an OP $C = 0 \rightarrow 1$ can be used to indicate the domains of different constituents’ particles, i.e., $C = 1$ indicates one particle phase while $C = 0$ denotes the other particle phase in an immiscible binary mixture. The interfacial region is tracked by $0 < C < 1$. The phase-field modeling approach has been successfully applied to explore the Ni particle coarsening associated with SOFCs evolution. For example, modeling work by Li et al.\textsuperscript{9} revealed that TPB area is significantly reduced due to the microstructural evolution of SOFC. Chen et al.\textsuperscript{30} quantitatively characterized the microstructural evolution by examining the TPB density, interfacial area, and tortuosity versus time using phase-field method. Abdeljawad et al.\textsuperscript{19} established an integrated phase-field model coupling the analysis of the microstructural coarsening process with SOFC electrochemical performance evaluation of SOFC. Many researchers, including but not limited to Aranson et al.,\textsuperscript{39} Karma et al.,\textsuperscript{40} Mieche et al.,\textsuperscript{41} and Marconi et al.\textsuperscript{42} have also explored crack formation using the phase-field model. Despite previous efforts, further investigation is yet to be done on long-term degradation of SOFC caused by microstructural evolution, which has been identified as one of the major sources of SOFC structural failure and performance degradation.\textsuperscript{20,30} Experimental investigation of SOFC electrodes degradation needs more further theoretical analysis.\textsuperscript{24} In particular, a more comprehensive understanding is needed to investigate the interplay between the dynamics of microstructural evolution at the meso-scale and electrochemical performance at the macro-scale.

In this work, a meso-scale computational framework was established to investigate the quantitative effect of Ni particle coarsening on the performance of SOFC. An integrated phase-field model was developed to couple microstructure evolution and crack formation in the anode. The developed meso-scale model captures the dynamics of Ni particle coarsening and crack formation in Ni-YSZ anodes. Moreover, it tracks the evolution of microstructural features that influence the electrochemical performance. The time-dependent microstructural properties obtained from the phase-field model was applied as effective properties to our previously developed SOFC electrochemical model\textsuperscript{1} to investigate the electrochemical performance of SOFC.

A graphical representation of performance degradation induced by SOFC microstructural evolution can be referred to Figure 1.

**Model Development**

In this work, SOFC anode consists of three constituents, Ni particle, YSZ, and pore. The mass of each phase inside anode is assumed to be unchanged. The modeling approach is based on the minimization of the total free energy of the anode that is represented by $F_{tot}$. YSZ is assumed to be stationary due to slow diffusion compared to Ni that evolves via diffusion along Ni-pore interface. Three OPs are utilized to represent Ni phase ($\xi$), YSZ phase ($\zeta$), and crack ($\Theta$), respectively. Based on the phase-field method, an OP changes continuously from 0 to 1 based on diffuse-interface theory. The range over which the OP changes from 0 to 1 is defined as interfacial region or interfacial thickness. For example, $\rho = 1$, $\rho = 0$, and $0 < \rho < 1$ represent the intact, fully broken, and the transitional interfacial thickness of the material. Minimization of total free energy leads to the interfacial diffusion. Interfacial diffusion can be formulated by using the Cahn–Hilliard equation as follows,

$$\frac{\partial \Theta}{\partial t} = M\nabla^2 \mu$$

where, $M$ is the mobility function that depends on the OPs of the system, $\nabla^2$ is the Laplace operator, and $\mu$ is the chemical potential of the system. The chemical potential is driven by total free energy that is based on dominant transport mechanism. The three phases of Ni-YSZ anode is considered immiscible, therefore, the effect of elastic energy is assumed to be negligible. $F_{tot}$ represent the total free energy of anode and can be expressed as follows,

$$F_{tot} = \int \left[ \frac{\Psi}{2} |\nabla \xi|^2 + f(\xi) + f(\Theta) + f(\sigma) \right] dV$$

where the first term on the right represents gradient energy, $\Psi$ donates interfacial thickness, $f(\Theta)$ is the fracture OP of anode, and $f(\sigma)$ is the elastic strain energy. $f(\cdot)$ is a generic double wall function that can be
represented as follows,

\[ f(\xi) = \frac{\xi^2 (1 - \xi^2)}{4} \]  

Eq. 6

Two boundary conditions (i.e., contact angle at the TPB and no flux at the Ni-YSZ interface) are implemented with the Cahn-Hilliard equation. No flux BC (i.e., \( \partial \mu \times \partial \xi = 0 \)) can be solved using the smoothed boundary method (SBM).\(^{43,44}\) The BC of contact angle is implemented as elaborated in the literatures.\(^{45,46}\) The Cahn-Hilliard equation for anode within SBM framework can be written as follows,

\[ \frac{\partial f}{\partial t} = - \nabla \cdot M(\xi, \dot{\xi}) \nabla \mu = \nabla \cdot \kappa \]  

where \( \kappa \) is the mobility function of two OPs (i.e., \( \xi \) and \( \dot{\xi} \)).\(^{40}\)

Karma et al.\(^{40}\) showed the choice of where \( \phi \) as follows,

\[ \phi = M(\xi, \dot{\xi}) \]  

The chemical potential of anode is denoted by \( \mu \) and can be represented by the following equation,\(^{46}\)

\[ \mu = \frac{\delta F_{an}}{\delta \xi} = f(\xi) - \phi^2 \nabla^2 \phi - g(\theta) \frac{1}{2} E \frac{\Omega}{2 - 2\Omega} \xi \]  

where \( \phi \) represents interfacial thickness, \( g(\theta) = \theta^3(4 - 3\theta) \), is the coupling function between the fracture OP and elastic stress field. Karma et al.\(^{40}\) showed the choice of \( g(\theta) \) does not affect the transport mechanism as long as \( g(\theta) = 0 \), \( \theta = 0 \) represents the material is fully fractured, \( E \) is the Young’s modulus, \( \nu \) is the Poisson’s ratio, and \( \Omega \) is the volume fraction of Ni phase (i.e., ratio of Ni volume to total anode volume).

Multiplying with the OP \( \xi \), Eq. 4 can be rewritten as follows,

\[ \frac{\partial (\xi \dot{\xi})}{\partial t} = \xi \nabla \cdot \kappa = \nabla \cdot (\xi \dot{\xi}) \]  

where \( \kappa \) represents characteristic length scale of sample, \( K_b \) is the Boltzmann constant, \( T \) is the temperature, \( N_s \) is the atomic number density, \( \delta_s \) is surface diffusin depth, \( \gamma_s \) is surface energy, and \( D_s \) is surface diffusivity.

In Eq. 12, \( M \) is the mobility function and can be formulated as follows,

\[ M(\xi, \dot{\xi}) = M_{Ni-pore} \prod \left( \xi^2 (1 - \xi^2) \right) g(\xi) \]  

where, \( g(\xi) \) is a function to control the Ni particle mobility near the TPB area, can be represented by a polynomial function,\(^{30}\)

\[ g(\xi) = \xi^6 \left( 10\xi^2 - 15\xi + 6 \right) \]  

(7)

The pores in anode are treated as pre-existing crack or initial cracks. Following the previous work,\(^{30}\) the governing equation for crack formation using fracture OP can be described as follows,

\[ \frac{1}{\omega} \frac{\partial \delta}{\partial t} = a \nabla^2 \theta - 32H \frac{\nabla \theta}{(1 - \theta)(1 - 2\theta) - 12 \delta^2 (1 - \theta)(\sigma - \sigma)} \]  

(15)

where, \( \omega \) is the relaxation constant, \( \theta \) is gradient energy co-efficient, \( H \) is the energy barrier,\(^{30}\) \( \delta \) is the elastic energy density, and \( \sigma \) is the threshold value strain.\(^{30}\)

The microstructural properties are expressed in non-dimensional units in order to allow the investigation with a wide range of particle size and particle size ratio. Suitable parameters of the mobility function are necessary for the effective calculation of the Ni particle coarsening process. Due to diffuse interface nature of the microstructure, it is necessary to get an asymptotic analysis of phase-field method for the normalization of time. Following the references,\(^{39,35,50}\) an asymptotic analysis has been developed to measure the characteristic time (time normalization),

\[ \tau = \frac{L^4 k_B T N_s}{\gamma_s D_s \delta_s} \]  

(16)

where, \( L \) represents characteristic length scale of sample, \( k_b \) is the Boltzmann constant, \( T \) is the temperature, \( N_s \) is the atomic number density, \( \delta_s \) is surface diffusin depth, \( \gamma_s \) is surface energy, and \( D_s \) is surface diffusivity.

Numerical Setup and Solver Flow

The simulations were carried out by solving governing Eqs. 12–15 in FeniCS, an open source finite element software. Numerical calculations were on the order of 884736 elements and required about 16 GB of RAM and 140 hrs of time when solved in parallel over seven cores on an Ubuntu Linux workstation with 24 3.4 GHz Intel Xeon processors. The numerical tolerance for convergence and tolerance for the Newton solver were both set to be \( 1 \times 10^{-6} \). The Newton iterative solver was utilized due to nonlinear nature of the governing equations. An open-source multiplatform tool ParaView was used for data analysis and visualization. The numerical solver flow can be referred to Figure 2.

Model Validation

The work focuses on the modeling of microstructural evolution in SOFC anode. Randomly dispersed Ni-YSZ anode was adopted for the simulations due to the difficulty of obtaining initial crystallographic orientation. Ni particle size of 0.55 \( \mu \)m and Ni-YSZ particle size ratio of 0.9 were used as initial values. Time step size for simulation represented one-hour operation in real time. The mobility for Cahn-Hilliard equation was taken as one. Simulation results show 26% increment in the Ni particle size after 1000 time steps, which agrees with the experimental result reported by Tanasini et al.\(^{24}\) Additionally, the particle size ratio of Ni-YSZ was decreased by 16%, while Tanasini et al.\(^{24}\) reported 14.6% decrement based on their experimental results.\(^{24}\) The comparison of model evolution shows a close match with the literature from Li et al.\(^{3}\) As for the volume ratios of three different phases, we used 30\% Ni phase, 30\% YSZ phase, and 40\% porosity to validate the simulation result obtained from the modeling work. Figure 4 shows the comparison of TPB evolution.
close match between the two simulation results for TPB fraction (i.e., TPB fraction is defined as the ratio between TPB volume and anode volume). The TPB area is calculated using the ParaView. The key model parameters and values are listed in Table I.

### Results and Discussion

In this work, the developed meso-scale phase-field model was applied to investigate the anode microstructural evolution and crack formation. The SOFC anode microstructure evolution is driven by the Ni particle coarsening process, which leads to TPB area reduction, long term performance degradation, and crack formation of SOFC. The developed model was also used to obtain the time dependent microstructural properties during microstructure evolution, which is later used to quantify the performance degradation of SOFC.

The temporal microstructural evolution in two-dimensional is shown in Figure 5. A randomly disordered microstructure is generated in a normalized domain, where blue color represents the Ni particle, green color represents the YSZ, and red color is the pore.

### Table I. Values of model parameters used in this study.

| Model parameter                  | Value          |
|----------------------------------|----------------|
| Elastic constant, GPa            | E              |
| Partial molar volume, m/mol      | \( \Omega \)   |
| Poisson ratio                    | P              |
| Energy barrier, J/m              | H              |
| Threshold strain \( \varepsilon \) | \( \epsilon \) |
| Characteristic length, m         | \( \psi \)     |
| Relaxation constant              | \( \omega \)   |
| Surface energy, J m\(^{-2}\)    | \( \gamma_s \) |
| Surface diffusion co-efficient, \( m^2 s^{-1} \) | \( D_s \) |
| Interfacial thickness, nm        | \( \delta \)   |
| Boltzmann constant, m\(^2\) kg \( s^{-2} \) \( K^{-1} \) | \( k_B \) |

\( E = 200 \)  
\( \Omega = 6.63 \times 10^{-6} \)  
\( P = 0.3 \)  
\( H = 5 \)  
\( \epsilon = 0.002 \)  
\( \psi = 25 \times 10^{-6} \)  
\( \omega = 0.3 \)  
\( \gamma_s = 1.9 \)  
\( D_s = 10^{-6} \)  
\( \delta = 1 \)  
\( k_B = 1.38 \times 10^{-23} \)
to explore the microstructural evolution process. During SOFC operation, the anode evolves over time due to coarsening of Ni particle. Due to the nature of diffusive interface, YSZ-pore phase interface and Ni-pore interface can be tracked with obtaining their microstructural parameters (e.g., particle size ratio, TPB fraction) by solving governing Eqs. 12–15. This particle coarsening process is driven by the minimization of total free energy, which causes average particle size to increase and the percolation connectivity to decrease. Two different stages of microstructures at $T = 40$ (i.e., 40 hrs operation) and $T = 1000$ (i.e., 1000 hrs operation) are shown in the figure.

The temporal three dimensional structural simulations are completed for the anode microstructure of 25 $\mu m \times 25 \mu m \times 25 \mu m$ with a mesh grid of $96 \times 96 \times 96$. The Ni-YSZ microstructure was generated following a previous study, where three phase volume fraction was prescribed as 27% Ni phase, 30% YSZ phase, and 43% pore phase. Figure 6 shows temporal three dimensional microstructural evolution for Ni, YSZ, and pore after 1000 hours of operation. Each of the constituents’ phases is shown in Figure 6. The simulation results show the internal structure of the connectivity of each phase, which can be utilized to quantify the growth of the average characteristic length and discriminate the percolated cluster from isolated clusters in the evolved anode.

Ni particle coarsening decreases TPB density and increases the resistance of anode. Figure 7 visualizes the reduction of the TPB area during the microstructural evolution process. The result shows, rapid reduction of TPB area at the initial stage of the coarsening process, which agrees with the experimental observation where the main performance change occurs at the initial stages. Due to high interfacial energy at the initial stages, the TPB area decreases rapidly, but it slows down over the time period. The TPB area reduction is consistent with the temporal phase coarsening, which indicates the performance degradation is directly related to the particle agglomeration and coarsening of Ni particle. The overall TPB area reduction is found to be approximately 24%, which is close to the experimental work of Cronin et al. 29

The evolution of pore phase has been illustrated in Figure 8. Numerous pores exist in anode to facilitate gas transportation. Pre-existing pores in Ni-YSZ grow due to interfacial diffusion during anode microstructure evolution which results in the increase of pore radius. By examining the evolution of pore phase, it can be concluded that the pores are growing in size and evolving into a more round shape, thus minimizing total free energy. The coupling effect of diffuse interface and stress evolution plays a vital role in the formation of cracks. Radius of the pore increases during the minimization of interfacial area. The interfacial diffusion during the evolution process leads to the accumulation of these expanded pores which causes crack formation. In the meanwhile, as Ni particle diffuses during microstructural evolution, the tensile stress field in the inner region evolves, which causes stress concentration at the crack tip. The stress concentration eventually leads to the formation of crack and subsequently structural failure. The simulation results are in good agreement with annealing experiments on Ni-YSZ anodes with Ni and YSZ particles of similar sizes, where a 25% decrease in total Ni-pore interfacial area was observed. 24

The temporal pore phase evolution is presented in Figure 9, which helps to visualize the crack formation during microstructural evolution in three dimension. Only the pore phase after the evolution is shown for an anode microstructure of 25 $\mu m \times 25 \mu m \times 25 \mu m$ with a mesh grid of $96 \times 96 \times 96$ to demonstrate crack formation. In the modeling work, the initial crack appears after 780 dimensionless time steps. Then, the crack formation develops quickly, as shown in Figure 9, at two different dimensionless time steps, $T = 40$ and $T = 1000$.

The microstructural features and effective material properties extracted from meso-scale phase-field simulations can be utilized to investigate the influence of Ni coarsening on the electrochemical performance degradation of SOFCs. For the electrochemical analysis in this section, we assigned an absolute value to the size of non-evolving YSZ particle as the characteristic length scale. In order to make the results as general as possible, all dimensions were scaled with respect to the characteristic length and no absolute physical dimensions of
Figure 7. Degradation of TPB during temporal evolution of three phase SOFC electrode at three different dimensionless time steps. (a) Time step = 40; (b) Time step = 500; (c) Time step = 1000 where the volume fractions are 27% Ni phase, 30% YSZ phase, and 43% pore phase at the initial stage.

Figure 8. Propagation of crack in the microstructure due to interfacial diffusion. (a) Blue, yellow, and red represent the Ni, YSZ, and pore, respectively at T = 40; (b) Formation of initial crack in microstructure at T = 780; (c) Propagation of crack due to the coupling effect of interfacial diffusion and stress evolution at T = 850.
the simulation box had been assigned. Peak power density plots are shown to quantify the performance degradation of SOFC due to microstructural evolution. Figure 10 compares the peak power density plot at the initial stage and after the degradation for an anode. The result shows, the peak density is 9550 W m\(^{-2}\) at the initial stage of the operation. However, the final peak power density decreases by 4.3% and reaches to 9150 W m\(^{-2}\) after the initial 500 hours of operation. After 1000 hours of operation the peak power density is further reduced to 8680 W m\(^{-2}\). Overall, 1000 hours of operation results in 9.11% decreased power output. However, the performance degradation appears to slow down during 500–1000 simulation time steps. The performance degradation is caused by the combined effects of continuous loss of TPB area, decrease in electronic conductivity, and the crack formation.

Figure 11 shows the performance degradation of anode supported SOFC due to crack formation. The formation of crack causes the interruption of current flow, which in turn increases the polarization resistance of the anode microstructure. The increased polarization resistance due to crack formation causes a sudden fall in the power density curve.\(^{54,55}\) The increase of polarization resistance is obtained from the experimental study.\(^{55}\) The peak power density at the initial stage of anode supported SOFC is 11345.34 W m\(^{-2}\). But the formation of cracks causes increased resistance and results in a 27% reduction in the peak power density and the obtained peak power density is 8210 W m\(^{-2}\).

Conclusions

A meso-scale phase-field model is developed to investigate performance degradation and crack formation during anode microstructural evolution. A phase-field model was developed to illustrate the effect...
of nickel particle coarsening in electrode microstructure. Randomly generated microstructure was considered and the time step size of 1 hour was used for the simulation. Developed phase-field model was validated against the experimental work by Tanasini et al. the modeling was used for the simulation. Developed phase-field model was validated against the experimental work by Tanasini et al. the modeling was used for the simulation.

The simulation result shows that the average particle size is increased during temporal microstructural evolution. The Ni particle size is increased by 26%, which leads to the TPB area reduction. Moreover, TPB phase contiguity is also affected significantly due to microstructural changes obtained from the phase-field simulation results are used as input parameter to the previously developed cell level model to quantify the performance degradation.

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List of Symbols

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| Symbol | Description |
|--------|-------------|
| $C_l$  | Lower cutoff order parameter value |
| $C_h$  | Upper cutoff order parameter value |
| $\delta$ | Surface diffusivity |
| $E$    | Young’s modulus |
| $F_{tot}$ | Total free energy |
| $H$    | Energy barrier |
| $k_B$  | Boltzmann constant |
| $k_e$  | Local curvature |
| $L$    | Characteristic length |
| $M$    | Mobility |
| $N_v$  | Atomic number density per volume |
| $n$    | Normal |
| $s$    | Surface |
| $T$    | Time (sec) |
| $V_e$  | Normal velocity |
| $V$    | Total volume |

Greek

| Symbol | Description |
|--------|-------------|
| $\alpha$ | Gradient energy coefficient |
| $\gamma_1$ | Surface energy |
| $\xi$   | Order parameter for Ni particle |
| $\xi_0$ | Order parameter for YSZ |
| $\phi$  | Order parameter for crack |
| $\varepsilon$ | Strain tensor |
| $\mu$  | Chemical potential of the anode |
| $\psi$  | Gradient energy coefficient |
| $\omega$ | Relaxation constant |
| $\sigma$ | Threshold strain |
| $\sigma_{ef}$ | Elastic energy density |
| $\delta_i$ | Interfacial thickness |
| $\psi$ | Poisson’s ratio (2011) |
| $\nu$ | Unit interface normal |
| $\Omega$ | Volume fraction of the phase |
| $\tau$ | Time scale for surface diffusion |

Operator

| Symbol | Description |
|--------|-------------|
| $\nabla^2$ | Laplacian |
| $\pi$  | Multiplication notation |
| $\delta/\delta s$ | Gradient operator along the interface |

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