Multilayer Interface Mathematics

Variational Method to Study Rapid Exchange in Multilayer Interfaces

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April 11, 2025

Abstract

This paper introduces a new branch of mathematics, multilayer interface mathematics. A mathematical model describing the energy of multilayer interfaces is constructed based on the variational method, which includes constructing the total energy functional from interface free energy, electrochemical energy, and diffusion transport energy. The corresponding Euler-Lagrange equations are derived. Each step of the mathematical derivation is explained in detail, clearly introducing how perturbation methods, the chain rule, and integration by parts are used to rigorously derive the target equations. The performance of fuel cells and lithium-ion batteries is largely limited by the rapid exchange efficiency of key ions in multilayer interfaces. Based on traditional models, we further introduce physical equations describing proton transport in hydrogen fuel cells and the rapid exchange of lithium ions in multilayer interfaces, providing quantitative design guidance for the fastest exchange of protons in fuel cell membrane electrodes and lithium ions in lithium-ion batteries through specific numerical examples and parameter sensitivity analysis.

Keywords: Fuel cells; Lithium-ion batteries; Multilayer interfaces; Variational method; Proton transport; Lithium-ion transport; Rapid exchange; Design optimization

1 Introduction

This paper introduces a new branch of mathematics, multilayer interface mathematics. A mathematical model describing the energy of multilayer interfaces is constructed based on the variational method. Fuel cells and lithium-ion batteries, as key technologies for clean energy and portable electronic devices, heavily rely on the transport efficiency of key ions in internal multilayer interfaces for their energy conversion efficiency and charge-discharge performance. In fuel cells, the proton transport speed in the membrane electrode directly affects energy conversion efficiency, while in lithium-ion batteries, the rapid passage of lithium ions in multilayer interfaces is crucial to the charge-discharge rate and energy density of the battery. Previous research has shown that by reasonably designing the thickness, chemical composition, and microstructure of each layer, the exchange rate of key ions can be significantly improved. This paper constructs the multilayer interface energy functional using the variational method and determines the optimal interface

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structure parameters based on energy minimization. We introduce physical equations describing ion transport, quantitatively studying the rapid exchange of key ions in fuel cells and lithium-ion batteries, and providing optimization guidance for practical designs.

2 Definition of Multilayer Interface Mathematics

Multilayer interface mathematics is an emerging branch of mathematics that specifically studies mathematical models and analysis methods for various physical, chemical, and electrochemical phenomena in interfaces composed of multiple functional layers. The field utilizes variational methods, partial differential equations, functional analysis, and numerical computation tools to construct and solve the total energy functional that describes interface free energy, electrochemical energy, and diffusion transport energy, thus deriving the Euler-Lagrange equations that reflect the equilibrium state of multilayer interfaces. Multilayer interface mathematics aims not only to reveal the essential mechanisms of internal interactions within multilayer interfaces but also to address the problem of achieving rapid exchange of key ions (such as protons in fuel cells and lithium ions in lithium-ion batteries) at interfaces, providing a rigorous theoretical foundation and quantitative design guidance for optimizing interface transport performance and enhancing device performance (such as proton transport in fuel cell membrane electrodes and lithium-ion charge-discharge processes). Additional features of multilayer interface mathematics will be published in subsequent works.

3 Theoretical Model and Construction of Energy Functional

3.1 System Description

In the multilayer interface region, each layer has different physical, chemical, and electrochemical properties, which directly determine the transport efficiency of key ions. Let $u(x)$ represent the spatial distribution of the interface structural parameters (such as functional group concentration or layer thickness distribution), where x is the spatial coordinate. At the same time, define the local potential $\phi(x)$ (assumed to be a known and continuous function). Together, these two parameters describe the energy state of the interface.

3.2 Construction of Total Energy Functional

To describe the entire multilayer interface system, we construct the total energy functional:

$$E[u] = \int_{\Omega} \Big[f_{\text{interface}}(u, \nabla u) + f_{\text{electrochemical}}(u, \phi) + f_{\text{diffusion}}(u, \nabla u) \Big] \, dx, \tag{1}$$

where:

- **Interface Free Energy Term:**

$$f_{\text{interface}}(u, \nabla u) = \frac{\gamma}{2} |\nabla u|^2 + V(u),$$

γ represents the interface tension, and $V(u)$ is the potential energy function reflecting the interaction between materials.

- **Electrochemical Energy Term:**

  $$f_{\text{electrochemical}}(u, \phi) = -q\, u\, \phi,$$

  where q represents the ion charge (positive for both protons and lithium ions).

- **Diffusion Transport Energy Term:**

  $$f_{\text{diffusion}}(u, \nabla u) = \frac{D}{2}|\nabla u|^2,$$

  where D is the effective diffusion coefficient.

Let $A = \gamma + D$, then the energy functional simplifies to:

$$E[u] = \int_\Omega \left(\frac{A}{2}|\nabla u|^2 + V(u) - q\, u\, \phi \right) dx. \tag{2}$$

4 Detailed Mathematical Derivation and Explanation

4.1 Perturbation Method and First-Order Variation

To find the extremum of $E[u]$, we perturb $u(x)$:

$$u(x) \to u(x) + \epsilon\eta(x),$$

where ϵ is a small parameter, and $\eta(x)$ is any smooth function satisfying the boundary condition (for example, $\eta(x) = 0$ at $\partial\Omega$). Substituting the perturbation into equation (2) and expanding to first order using Taylor's expansion, we get:

$$E[u + \epsilon\eta] = \int_\Omega \left\{ f(u, \nabla u) + \epsilon \left[\frac{\partial f}{\partial u}\eta + \frac{\partial f}{\partial(\nabla u)} \cdot \nabla\eta \right] + O(\epsilon^2) \right\} dx.$$

Thus, the first-order variation is defined as:

$$\delta E = \left.\frac{dE}{d\epsilon}\right|_{\epsilon=0} = \int_\Omega \left[\frac{\partial f}{\partial u}\eta + \frac{\partial f}{\partial(\nabla u)} \cdot \nabla\eta \right] dx. \tag{3}$$

Note: The higher-order term $O(\epsilon^2)$ is ignored, and the Taylor expansion and linearization method are standard steps in variational analysis.

4.2 Partial Derivatives Calculation

4.2.1 Partial Derivative with Respect to u

From

$$f(u, \nabla u) = \frac{A}{2}|\nabla u|^2 + V(u) - q\, u\, \phi,$$

only $V(u)$ and $-q\, u\, \phi$ depend on u, so we have:

$$\frac{\partial f}{\partial u} = V'(u) - q\, \phi.$$

Note: $V'(u)$ is the derivative of $V(u)$ with respect to u, and the derivative of $-q\, u\, \phi$ with respect to u is $-q\, \phi$.

4.2.2 Partial Derivative with Respect to ∇u

For the gradient term, we have:

$$\frac{\partial}{\partial(\nabla u)}\left(\frac{A}{2}|\nabla u|^2\right) = A\,\nabla u.$$

The other terms do not depend on ∇u, so:

$$\frac{\partial f}{\partial(\nabla u)} = A\,\nabla u.$$

Note: This is obtained using the chain rule and the formula for the derivative of the dot product.

4.3 Integration by Parts and Euler-Lagrange Equation

Substituting the above results into equation (3), we get:

$$\delta E = \int_\Omega \left[(V'(u) - q\,\phi)\,\eta + A\,\nabla u \cdot \nabla\eta\right] dx.$$

Applying integration by parts to the second term (assuming $\eta(x)$ is zero on the boundary):

$$\int_\Omega A\,\nabla u \cdot \nabla\eta\,dx = -\int_\Omega A\,\Delta u\,\eta\,dx.$$

Thus, the variation becomes:

$$\delta E = \int_\Omega \left[V'(u) - q\,\phi - A\,\Delta u\right]\eta\,dx. \tag{4}$$

By the fundamental lemma of variational calculus, since $\eta(x)$ is arbitrary, we must have:

$$V'(u) - q\,\phi - A\,\Delta u = 0. \tag{5}$$

Note: According to the basic variational principle, if for all smooth test functions $\eta(x)$, we have $\int_\Omega G(x)\eta(x)dx = 0$, then $G(x) = 0$. Hence, we obtain the Euler-Lagrange equation, which describes the interface structure that extremizes the energy functional.

5 Applications of the Variational Method to Rapid Ion Exchange

One innovative aspect of this paper is the use of the variational method to study the rapid exchange of key ions in multilayer interfaces, thereby optimizing design.

5.1 Rapid Exchange of Protons in Fuel Cell Membrane Electrodes

In fuel cells, the rate of proton transport in the membrane electrode directly determines energy conversion efficiency. By optimizing $u(x)$ and controlling the potential function $V(u)$ to minimize the local energy barrier, we accelerate proton transport. When the condition

$$V'(u) \approx q\,\phi + A\,\Delta u, \tag{6}$$

is satisfied, the optimal transport channel can be constructed, enabling the fastest exchange of protons.

5.2 Rapid Transport of Lithium Ions in Multilayer Interfaces

For lithium-ion batteries, the exchange rate of lithium ions in multilayer interfaces is equally important. Similarly, the energy functional constructed using the variational method applies to lithium ions, where q represents the charge of lithium ions. When the condition

$$V'(u) \approx q\,\phi + A\,\Delta u, \tag{7}$$

is satisfied, the transmission energy barrier for lithium ions in the interface is minimized, achieving the fastest passage of lithium ions and thus improving charge-discharge performance and energy density.

6 Specific Numerical Calculation Examples

Below, we quantitatively estimate key parameters for hydrogen fuel cells and discuss similar applications for lithium-ion systems.

6.1 Proton Mobility and Conductivity Calculation

Using the Einstein relation:

$$\mu_{\text{eff}} = \frac{q\,D_{\text{eff}}}{k_B T}.$$

Take the following parameters:

$$q = 1.602 \times 10^{-19}\,\text{C}, \quad D_{\text{eff}} = 5 \times 10^{-10}\,\text{m}^2/\text{s},$$

$$k_B = 1.38 \times 10^{-23}\,\text{J/K}, \quad T = 353\,\text{K}.$$

Substituting these values, we get:

$$\mu_{\text{eff}} \approx 1.64 \times 10^{-8}\,\text{m}^2/(\text{V} \cdot \text{s}).$$

Next, assume the proton concentration $c = 1 \times 10^{26}\,\text{m}^{-3}$:

$$\sigma_{\text{eff}} = 1.602 \times 10^{-19} \times 1 \times 10^{26} \times 1.64 \times 10^{-8} \approx 0.26\,\text{S/m}.$$

Note: These calculations use standard physical constants and experimental parameters to derive the proton mobility and conductivity, which serve as a reliable data foundation for subsequent proton flux estimates.

6.2 Proton Flux Estimation

Assuming the interface potential difference $\Delta\phi = 0.5\,\text{V}$, the effective thickness of the interface $d = 10\,\mu\text{m} = 1 \times 10^{-5}\,\text{m}$:

$$J \approx 0.26\,\text{S/m} \times \frac{0.5\,\text{V}}{1 \times 10^{-5}\,\text{m}} \approx 1.3 \times 10^{4}\,\text{A/m}^2.$$

Note: This estimation uses Ohm's law to approximate the proton flux, linking the interface conductivity, geometry, and potential difference.

6.3 Discussion on Lithium-Ion Systems

For lithium-ion batteries, although specific parameters (such as diffusion coefficient D_{eff} and concentration c) may differ, the basic mathematical model and variational method apply similarly. After obtaining suitable experimental parameters, $u(x)$ can be adjusted to satisfy the condition

$$V'(u) \approx q\,\phi + A\,\Delta u,$$

to achieve the fastest transport of lithium ions in multilayer interfaces, thus improving the battery's charge-discharge rate and energy density.

7 Numerical Simulation and Discussion

7.1 Parameter Sensitivity Analysis

Through numerical simulations, we can evaluate the impact of the following key parameters on interface structure and ion transport efficiency:

- **Interface Layer Thickness (d):** Thinner, uniform layers help reduce energy loss due to potential gradient and optimize ion exchange rate.
- **Potential Function $V(u)$:** By designing appropriate functional groups to control the shape of $V'(u)$, local potential distribution can be optimized, reducing the ion exchange barrier.
- **Electrochemical Term ($q\,\phi$):** The applied potential and its gradient directly drive ion migration, significantly affecting the exchange rate.
- **Effective Diffusion Coefficient (D_{eff}):** Closely related to the microstructure of the interface material, it plays a decisive role in ion diffusion performance.

7.2 Numerical Solution Methods

For the Euler-Lagrange equation

$$-A\,\Delta u + V'(u) - q\,\phi = 0,$$

we can discretize it using finite element or finite difference methods, combined with Newton's iterative method to solve the nonlinear equation system. Further, by coupling the Nernst-Planck equation and the electric field distribution, a multi-physics model can be constructed to determine the optimal interface structure parameters. **Note:** Numerical solution methods make solving complex partial differential equations possible, and through sensitivity analysis, design parameters can be further optimized to achieve the best ion exchange effects.

8 Practical Design Guidance

Based on the above theoretical models and numerical calculations, this paper proposes the following design recommendations:

1. **Optimize rapid ion exchange:** By optimizing interface structure using the variational method, protons and lithium ions can exchange at the fastest rate in multilayer interfaces, which is critical for improving the performance of fuel cells and lithium-ion batteries.

2. **Proton rapid transport in fuel cell membrane electrodes:** Based on equation (6) and numerical calculations, the interface conductivity σ_{eff} should be increased (i.e., increasing local proton concentration c and mobility μ_{eff}), and the effective thickness d should be reduced to achieve the fastest proton transport.

3. **Rapid transport of lithium ions in multilayer interfaces:** Similarly, by adjusting the interface structure and chemical functional groups to satisfy equation (7), the ion transport barrier for lithium ions can be minimized, thus improving the battery's charge-discharge rate.

4. **Multi-scale collaborative design:** At the nanoscale, improve ion transport performance by modifying the local chemical structure; at the macroscale, reduce interface resistance through overall structural design, achieving the best design parameters with synergistic effects.

5. **Ensure durability and stability:** While optimizing rapid exchange efficiency, it is crucial to balance thermal, moisture, and mechanical stability for the long-term reliable operation of fuel cells and lithium-ion batteries.

9 Conclusion

This paper constructs the energy functional model of hydrogen fuel cells and lithium-ion multilayer interfaces based on the variational method and derives the corresponding Euler-Lagrange equations. Based on the Einstein relation and the Nernst-Planck equation, the rapid exchange of protons and lithium ions is systematically analyzed through mathematical derivation and quantitative calculations. Numerical simulations and parameter sensitivity analysis show that optimizing interface layer thickness, functional group distribution, and local potential distribution can significantly reduce ion transport barriers, improve the exchange rate of key ions, and provide solid theoretical and quantitative support for the design of fuel cells and lithium-ion batteries.

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