Dynamics of Oxygen Scattering on Ionomer Surface in Catalyst Layer of PEFC

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Background

Polymer Electrolyte Fuel Cell (PEFC)

Important issues for utilization
- High current density operation
- Low weight and volume
- Cost reduction

The cell performance degrades with increasing the current density.

H₂→2H⁺+2e⁻ (Anode)
O₂+2H⁺+2e⁻→H₂O (Cathode)

Oxygen transport is one of the important factors.
- Transport in Catalyst layer (CL)
- Transport in Microporous layer (MPL)

Intermediate region between the Knudsen and molecular diffusion.

Objectives

To understand the oxygen transport in nanoscale structure of scattering phenomena in PEFC

Direct Simulation Monte Carlo (DSMC)
- Effective method to analyze gas transport in nanoscale structure.
- An accurate scattering model is required.

Investigate the scattering dynamics on ionomer surface using molecular dynamics simulations

Simulation system

Polymer chain (Nafion) - 4 chains
- Chemical structure of Nafion

Solvant molecules (H₂O + H₂O)
- N₁₅₀ = 40 (= N₂₀₂)
- Water contents j = 3, 7, 11 (= N₂₆₆/N₂₀₂)
- 3,000 trajectories for each incident conditions.

Incident condition

Incident translational energy Eᵢ₃ = 0.447, 0.894, 1.34, 1.79 kcal/mol

Incident angle θᵢ₃ = 0, 30, 60° (with respect to the surface normal)

Conclusions

Investigate the scattering dynamics on ionomer surface using molecular dynamics simulations

- Energy distributions depend on the incident energy and differ from the Maxwell–Boltzmann distribution.
- Reflection retaining the effect of incident energy.
- Angular distributions show good agreement with the cosine reflection law.
- Diffusive reflection on ionomer surface.
- Fraction of TD increases with increasing water content and normal component of incident energy.
- The surface diffusion becomes more important.

This work was supported by the New Energy and Industrial Technology Development Organization (NEDO) of Japan.
Our calculations were supported by the supercomputer system of Institute of Fluid Science, Tohoku University in Japan.

Energy distribution

As incident energy increases
- Shift to higher value
- Broader distribution

Diffusion reflection model
The scattering molecules obey
- Maxwell–Boltzmann velocity distribution at the surface temperature
- Cosine reflection law

Angular distribution

Evaluation of scattering events by angle
- Scattering angle θₙ respect to surface normal
- Azimuthal angle φₙ angle between incident and reflect vectors

Angular distributions show good agreement with cosine reflection law.
Oxygen molecules are reflected diffusely on ionomer surface.

Inelastic scattering (IS) and trapping desorption (TD)

Fraction of TD increases as the incident angle decreases.
The surface diffusion becomes more important.

Results and Discussion

Energy distribution

Fraction of TD

incident angle θᵢ₃ [deg.]

As incident energy increases
- Shift to higher value
- Broader distribution

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