BT04

Hydrogen Transport through Fractal Hydride-Forming Electrode: Current Transient Analysis by Monte-Carlo Simulation

프랙탈 형상의 수소화물 형성 전극을 통한 수소 이동에 관한 연구: 몬테 카를로 시뮬레이션을 이용한 전류 추이 곡선의 해석

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Hydrogen transport through the fractal hydride-forming electrode was theoretically investigated by analysis of the potentiostatic current transient using Monte-Carlo simulation. The fractal profiles were constructed with various values of the self-affine fractal dimension from the Weierstrass function, and then the current transients were simulated under the constraint by Butler-Volmer behaviour, i.e. the constraint of hydrogen diffusion mixed with interfacial charge transfer. The simulated current transients hardly followed the generalised Cottrell behaviour, and especially they exhibited an inflexion point at the time that corresponds to the temporal outer cut-off of fractality τ_0. As the potential step and the conversion factor representing the rate constant of charge transfer increased, the current decayed more rapidly with time until τ_0 was encountered. From the fact that the larger the values of both simulation parameters were, the shorter appeared τ_0, it was also suggested that the temporal cut-off range of fractality under the constraint by Butler-Volmer behaviour is not determined only by the spatial cut-off range and the hydrogen diffusivity in the electrode, but also by the magnitude of potential step and the rate constant of charge transfer. The anodic current transients were experimentally measured from the fractal Pd electrode obtained by a repetitive oxidation-reduction cycling, and subsequently they were analysed with the aid of the theoretical current transients.

References

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