BT03

Lithium Transport through Partially Inactive Transition Metal Oxide Electrode in Terms of Fractal Geometry: Current Transient Analysis by Monte Carlo simulation

프랙탈 기하학을 이용한 부분적으로 비활성된 전이금속 산화물 전극을 통한 리튬 이동에 관한 연구: 몬테 카를로 시뮬레이션을 이용한 전류 추이 곡선의 해석

정규남 · 변수일
한국과학기술원 신소재공학과

Lithium transport through partially inactive transition metal oxide electrode was theoretically investigated by analysis of the potentiostatic current transient using Monte Carlo simulation in terms of fractal geometry. The partially inactive surfaces with various values of the fractal dimension were constructed from the Cantor bar, and then the current transients were simulated under the cell-impedance-controlled constraint, i.e. lithium transport is limited by the internal cell resistance coupled with the lithium diffusion in the electrode. The simulated current transients hardly followed the generalised Cottrell behaviour, and especially they exhibited an inflection point at the time that corresponds to the temporal outer cut-off of fractality τ_o. As the conversion factor representing the internal cell resistance decreased, the current decayed more rapidly with time until τ_o was encountered. From the fact that the smaller the values of the conversion factor were, the shorter appeared τ_o, it was also suggested that the temporal cut-off range of fractality under the cell-impedance-controlled lithium transport is not determined only by the spatial cut-off range and the lithium diffusivity in the electrode, but also by the internal cell resistance. The anodic current transients were experimentally measured from the binder-dispersed $LiMn_2O_4$ composite electrode, and subsequently they were analysed with the aid of the theoretical current transients.

References

1. J.-W. Lee and S.-I. Pyun, Electrochim. Acta, 50 (2005) 1947.
2. J.-Y. Go and S.-I. Pyun, press in Electrochim. Acta (2005).