

Phase field modelling of the phase transformation kinetics of lithium inserted anatase TiO₂

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TiO₂ anatase is a promising negative electrode for lithium ion battery due to its high reversible capacity, chemical safety and environmental friendly properties. The phase transformation behavior of lithiated anatase TiO₂ had been intensively studied from the experimental point of view. Phase field modelling has recently exhibited good ability to capture experimental phenomenon for TiO₂ anatase upon lithiation. We performed DFT energy calculation and Monte Carlo simulation to obtain the Gibbs free energy curve, making this simulation more close to the physics of lithium inserted anatase TiO₂. On this basis, the phase field modelling is used to explore the comprehensive physics picture of the non-equilibrium phase transformation behavior that we firstly found in TiO₂ anatase upon lithiation by in-situ X-ray diffraction.