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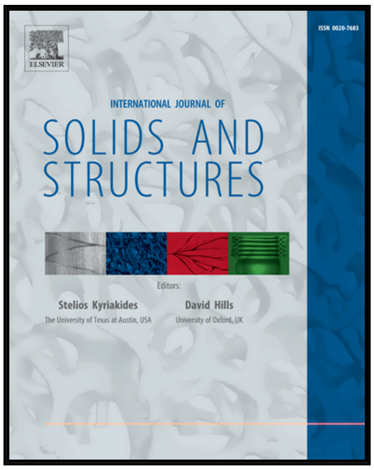

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Large Deformation Analysis of Diffusion-Induced Buckling of Nanowires in Lithium-Ion Batteries

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Abstract: Buckling due to diffusion-induced compressive stress has been observed during the lithiation of various nanowires, and can affect the mechanical and electrochemical performance of nanowire-based electrodes. This study is focused on the diffusion-induced buckling of nanowires. Two diffusion paths are analyzed; one with radial diffusion only, and the other with axial diffusion. For the diffusion-induced buckling of nanowires with radial diffusion, the theory of large deformation is used in the description of the coupling between mass transport and deformation in large deformed solids. Using the linear theory, analytical solution of the critical length of a nanowire, below which there is no buckling, is obtained, which is dependent on the constraint of the ends of the nanowire and the volumetric strain of the nanowire at the fully lithiated state. The comparison between the linear analytical solution of the critical length and the numerical solution from the theory of large deformation shows that the linear analytical solution is valid for the influx less than 1 $mol{\cdot}m^{-2}{\cdot}s^{-1}$ and configurations considered in the work. Numerical analysis shows that the critical buckling time decreases with the increase of nanowire length and current density, and the nanowire