

Supporting Information:

Computational analysis of chemomechanical behaviors of composite electrodes in Li-ion batteries

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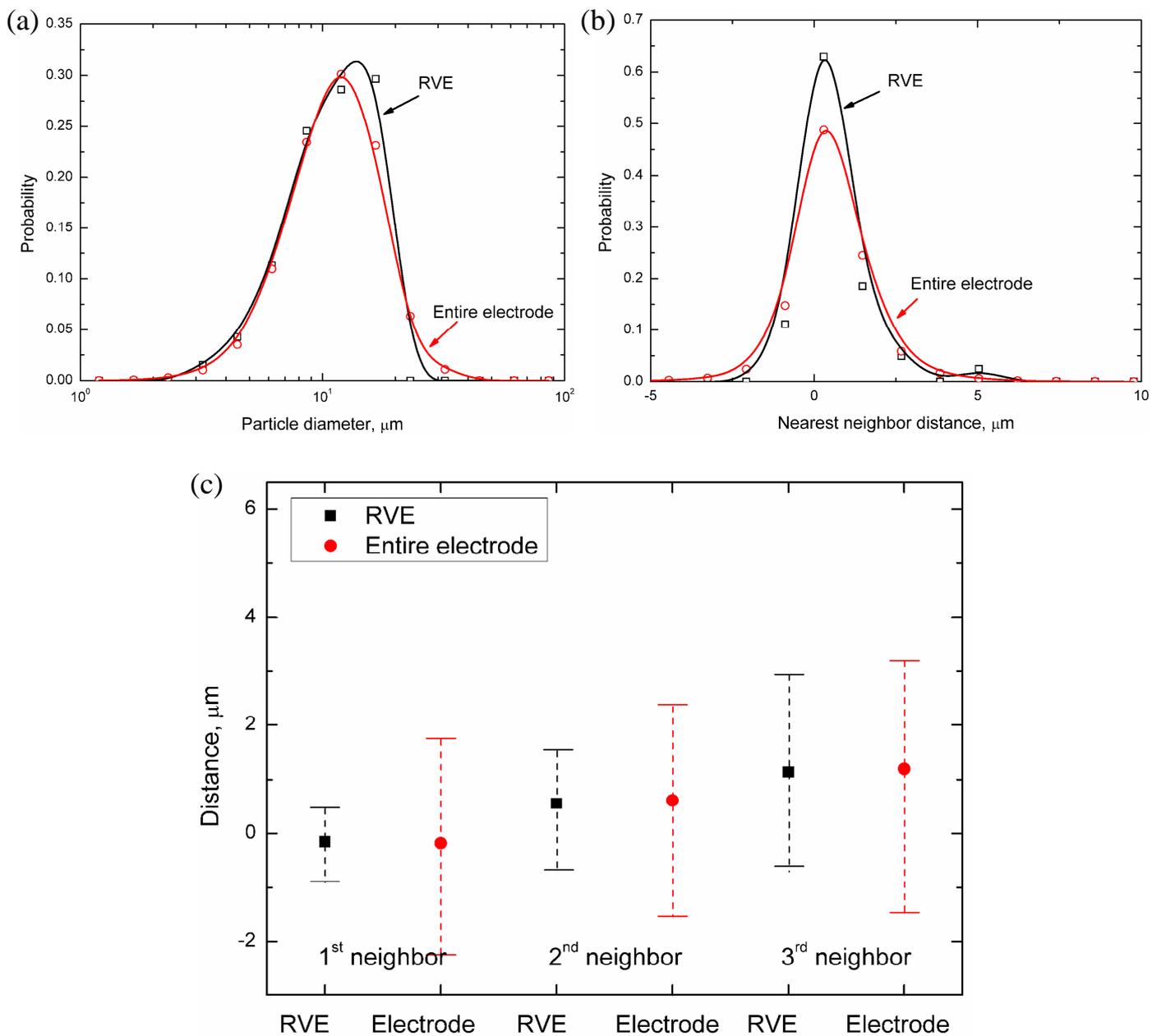


Fig. S1. Statistical analysis of (a) particle size distribution, (b) distance between the nearest neighboring particles, and (c) distance from the 1st, 2nd, and 3rd neighbor for individual particles in the RVE of compressed NMC electrodes.

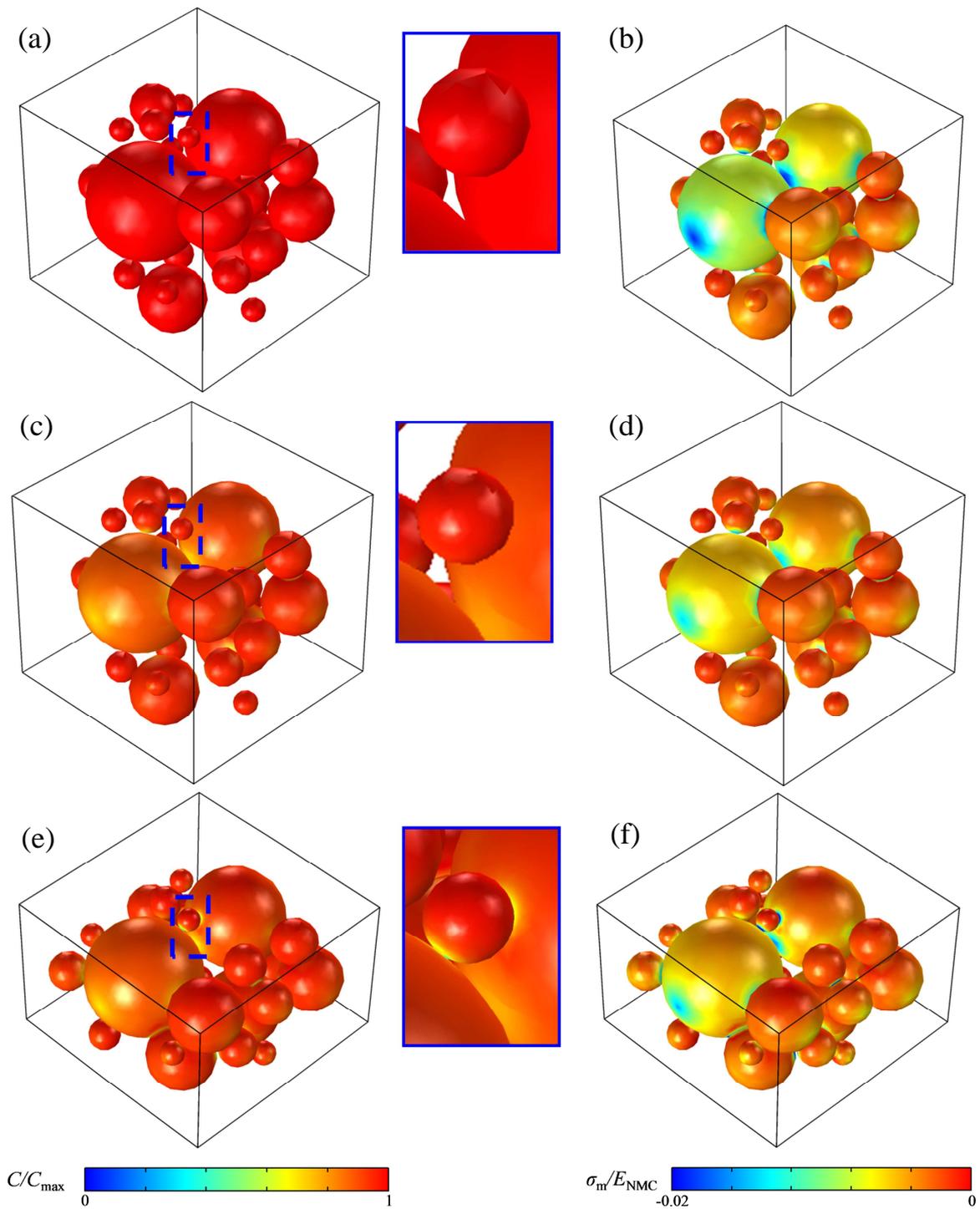


Fig. S2. The left column shows the Li profiles at the fully lithiated state ($Dt/A^2=1$) after potentiostatic lithiation of the uncompressed RVE without (a) and with (c) the stress effect, and of the compressed RVE with the stress effect (e), respectively. The right column ((b), (d), and (f)) shows the corresponding distribution of mean stresses. The mechanical interactions among the particles (local view in the middle column) regulate Li distribution and the large compressive stresses impede Li insertion into the particles.

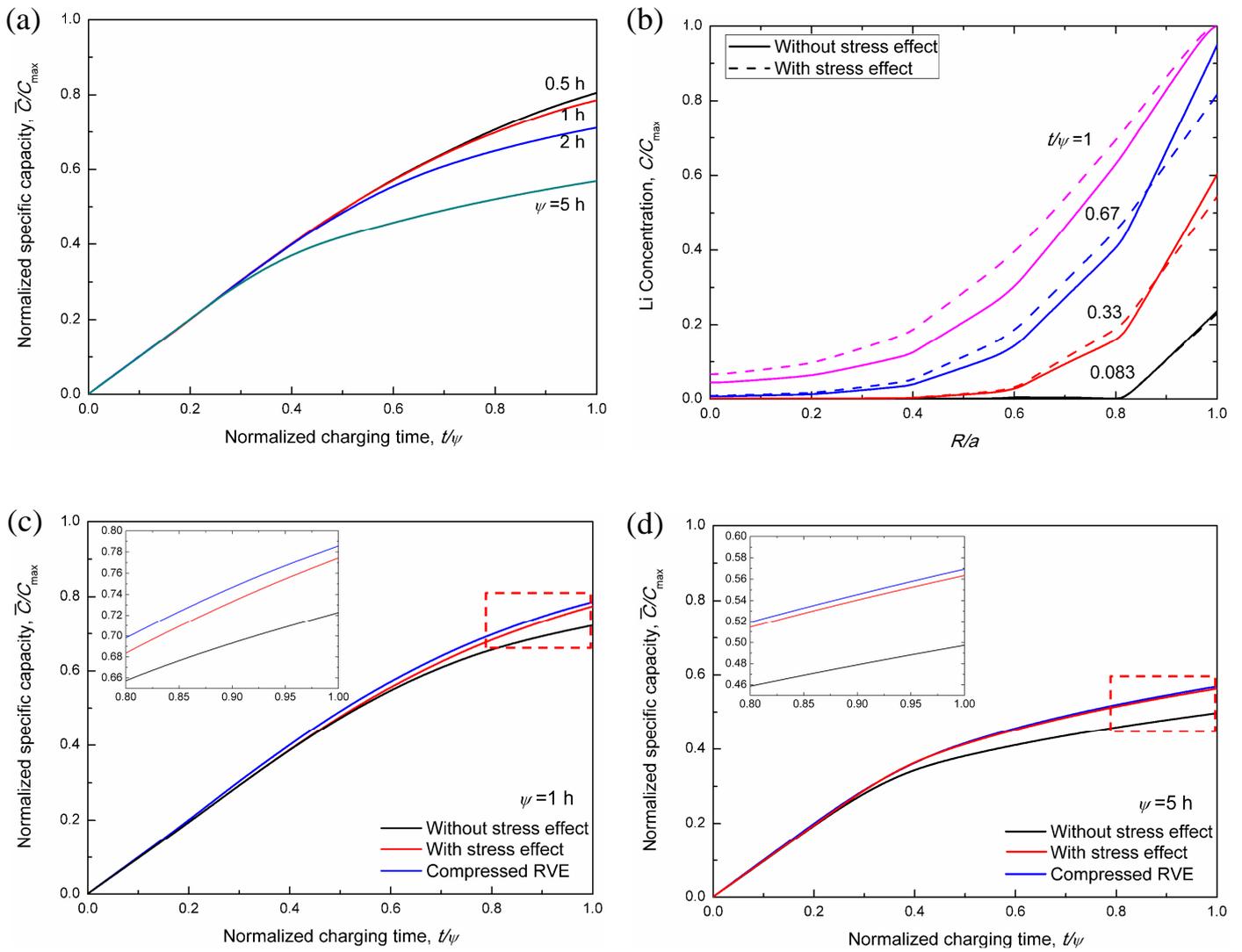


Fig. S3. (a) Specific capacity of the composite electrode lithiated at different galvanostatic rates. (b) Li concentration profiles in the composite electrode at different time steps of galvanostatic lithiation. (c) and (d) The influence of stresses on the specific capacity of the composite electrode for the galvanostatic lithiation rate $\varphi = 1$ h and $\varphi = 5$ h, respectively.