Supplementary Information (SI) for Journal of Materials Chemistry A.

Supplementary information for

Investigation of charge transfer models on the evolution of phases in lithium iron phosphate batteries using phase-field simulations

Souzan Hammadi,[a] Peter Broqvist,[a] Daniel Brandell[a] and Nana Ofori-Opoku[b]

[a] Department of Chemistry – Ångström Laboratory, Uppsala University, 75121 Uppsala, Sweden
[b] Department of Materials Science and Engineering and Brockhouse Institute for Materials Research, McMaster University, Hamilton, L8S 1L4, Canada

Stiffness matrix

The elements in the stiffness matrix are,

$$C_{11} = \lambda\frac{1-\nu}{\nu}, \quad C_{12} = \lambda \quad \text{and} \quad C_{44} = \lambda\frac{1-2\nu}{2\nu}. \tag{1}$$

The Lamé constant, λ, is defined using Poisson's ratio, ν, and Young's modulus, E,

$$\lambda = \frac{E\nu}{((1+\nu)(1-2\nu))}. \tag{2}$$

The stiffness matrix is thus defined as,

$$C_{2D} = \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & C_{44} \end{bmatrix} \tag{3}$$

$$C_{3D} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} \tag{4}$$

3D simulations

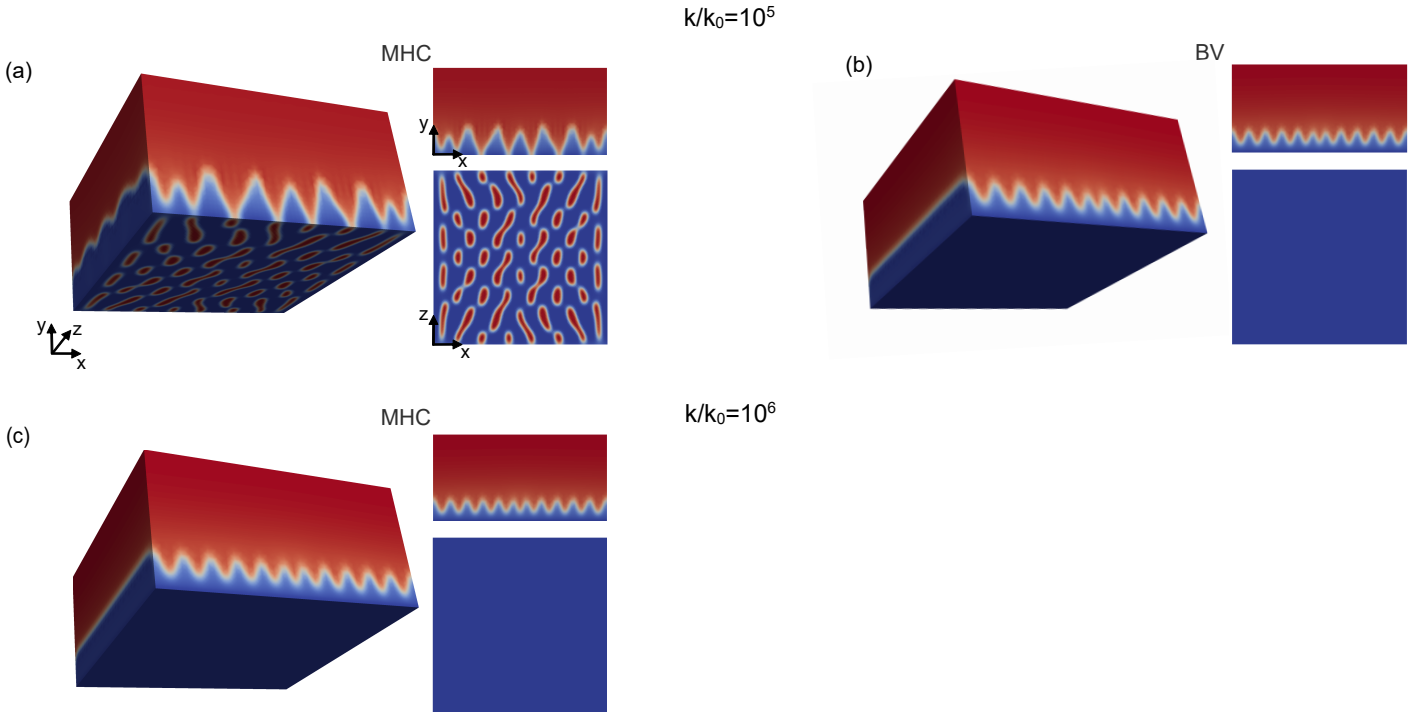

Figure 1 Snapshots of 3D simulations with MHC and BV, at 80 % Li corresponding to Figure 7 in the paper.

2D simulations

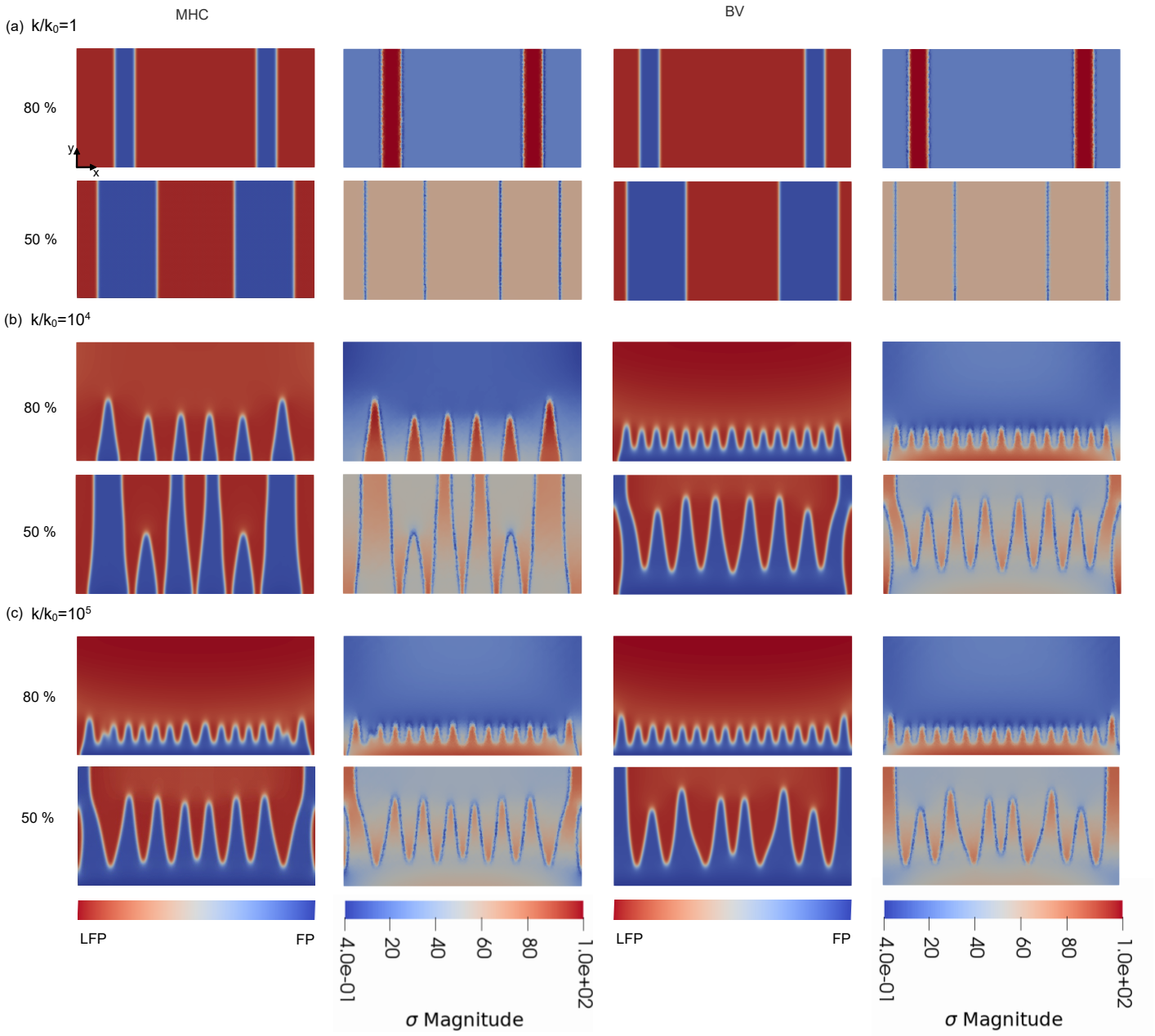

Figure 2 Snapshots corresponding to the 2D simulations presented in Figure 5 in the paper, at 80 and 50 % Li, $\Delta\Phi$=100 mV applied potential. Showing the evolution of concentration and stress (σ) magnitude for simulations using Butler-Volmer and Marcus-Hush-Chidsey charge transfer reaction models.