Multiscale modeling of diffusion in elastic composite materials

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Our research features diffusion in elastically deformable solids with complex microstructure. A prominent example are electrodes of Li-ion batteries which are typically a porous compound consisting of a binder, conductive particles, and active particles, filled with an electrolyte. The charge and discharge processes are complex multi-physics problems. Based on the used materials, they may include chemical reactions, electrochemically driven diffusion, separation into lithium poor and lithium rich regions in the active particles, or swelling phenomena [1]. Here, we consider a simplified version of this problem restricting ourselves to diffusion in an elastic matrix-particle composite. In the matrix, the transport of the mobile species is described using a Fickian-type flux driven by the gradient of the chemical potential. In the particles, the mobile species tends to accumulate and build separate regions of equal concentration – either high or low. This behavior is modeled using the Cahn-Hilliard equation.

When the dimensions of the computational domain increase, it is less surprising that a direct numerical simulation is computationally extremely demanding. To circumvent this difficulty, an extended version of the computational homogenization procedure presented in [2] is employed. There, instead of modeling the body in full detail, a homogenized problem is considered. The unknown constitutive response, such as the species flux or the stress tensor, is computed from the known constitutive response of a statistically representative volume element. The coupling of the homogenized macroscopic problem with the representative microscopic problem is achieved via appropriate boundary conditions. The figure below compares the results of a direct numerical simulation with the homogenized solution. Both relevant cases, diffusion driven deformation and deformation driven diffusion, are studied. First a flux is prescribed on the left boundary. Afterwards the top left half of the body is loaded with a constant force per length. As can be seen, in the particles, the mobile species creates regions of high (red) or low concentration (blue) whereas in the matrix, the concentration field is rather homogeneous. The body expands at high concentrations and contracts at low concentrations. Under pressure, the particles prefer a low species concentration.

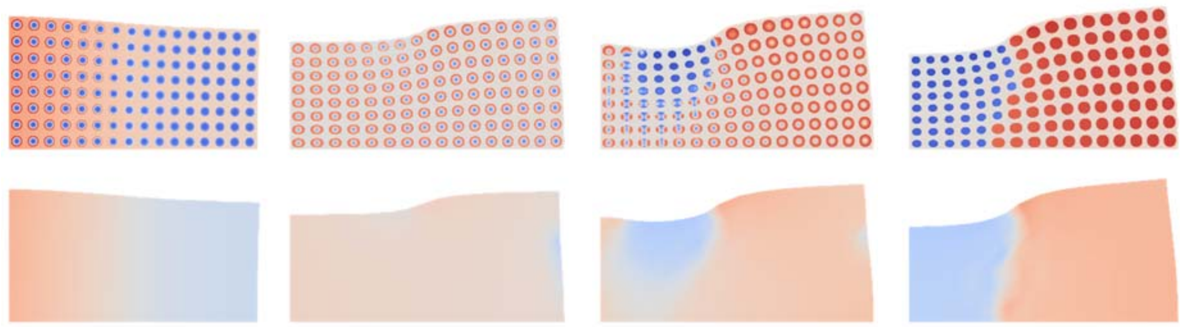

Figure 1: Deformation driven diffusion in a matrix particle composite.

References

[1] D. Grazioli, M. Magri, A. Salvadori: *Computational modeling of li-ion batteries*. Computational Mechanics **58**(6), 889-909 (2016).

[2] S. Kaessmair, P. Steinmann: *Computational first-order homogenization in chemomechanics*. Archive of Applied Mechanics **88**(1-2), 271-286 (2018).