Modelling Panel Abstract & Speaker Biography

Reaction kinetics and diffusion-migration processes in an idealised lithium-sulfur cell

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The behaviour of a Lithium-sulfur (LiS) cell depends on a complex mix of species interactions, as solid-phase sulfur S_8 is reduced to solid-phase lithium sulfide Li_2S via a series of chemical and electrochemical reaction processes in the solvent phase. The exact mechanism is unknown and is furthermore difficult to identify experimentally, although a number of reaction pathways have been proposed[1].

In order to help understand the system, modelling provides a useful second route to identify the likely processes driving the cell during its operation. Structurally, a Li-S cell has a metal anode, a porous separator and a porous sulfur-containing carbon-based cathode. A common modelling approach is to homogenise the porous structures of the cell and to solve for the diffusion-reaction processes occurring within them using the Nernst-Planck equation coupled to the Butler-Volmer equation, under the assumption of electroneutrality[2].

While this homogenisation approach has proven useful and leads to reasonable cell scale models[3], an underlying problem with them is that the electrolyte concentrations, cell operating potentials and species charges mean that the dilute solution theory upon which the models are based is inaccurate[4,5]. In particular, the complexity of the electrolyte means that the interfacial region between the electrode and the electrolyte – the electric double layer – is poorly described by these models. Since most processes occurring in a Li-S cell take place in this region, it is important to understand whether incorporating a better description of it can improve our knowledge of the microscopic cell behaviour.

In this talk we will discuss the development of a model based on a non-electroneutral, modified dilute solution theory and how we are using this to try and further understand the reaction mechanism of a Li-S cell. The resulting one-dimensional model describes diffusion-migration, surface electrochemical reactions, surface chemical reactions (precipitation/dissolution) and bulk phase chemical reactions (association/dissociation) in an idealised cell structure. The result is a useful tool for investigating the emergent behaviour of complex reaction-diffusion-migration systems.

References

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Speaker Biography:

Dr Geraint Minton graduated in 2014 with a PhD in Electrochemistry from the University of Manchester. His research focussed on the theoretical study of how species interactions affect both the equilibrium state and dynamic behaviour of electrode-electrolyte systems, in particular looking at the electric double layer and how changes in its structure affect the macroscopic properties of the overall system.

Since graduating he has been working for OXIS Energy as part of the Revolutionary Electric Vehicle Battery (REVB) project, using these methods and others to develop models to help understand the complex processes underlying the behaviour of lithium-sulfur cells.

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