Generation and mechanical characterization of particulate coatings via DEM simulations - An application to Lithium-ion battery electrodes

Clara Sangrós Giménez[*], Carsten Schilde[*] and Arno Kwade[*]

[*] Institut für Partikeltechnik
Technische Universität Braunschweig
Volkmaroderstraße 5, 38104 Braunschweig (Germany)
e-mail: c.sangros@tu-braunschweig.de, web page: http://www.ipat.tu-bs.de/

ABSTRACT

Microstructural characteristics of particulate coatings such as porosity and particle size distribution are of major importance in determining their bulk properties. For instance, the performance of a lithium-ion battery can be significantly enhanced by selecting the adequate electrode porosity or by adjusting the correct amount of binder.

Within this framework, the present study proposes a discrete element method (DEM) procedure to create particulate coatings with defined product characteristics and to give insight into the influence of microstructure with regard to the mechanics. Operating the open source software LIGGGHTS with additional programming code, particulate structures can be computer generated taking into consideration specific particle size distribution, bulk porosity and coating thickness. This process is automatized and fulfilled by an iterative adjustment of input parameters. The application of this effective designed tool is put into practice for the numerical generation of lithium-ion electrode structures. These composite materials consist of active material and conductive additive particles combined with a binder, which ensures the cohesion throughout the particulate network and the adhesion between the coating and the substrate. The role of the binder in the mechanics of the system is therefore essential and must also be considered for the simulations. Bearing this fact in mind, a Hertzian-bond contact model was also developed in this study in order to capture the elasto-plastic behavior of the electrode. This contact model combines both particle and binder stiffness by computing bonds between particles under certain conditions with regard to interparticle distance and particle radii.

Within this work, different electrodes were experimentally produced as well as numerically generated in order to validate the implemented procedure. Furthermore, nanoindentation experiments and corresponding simulations were carried out with the aim of calibrating and validating the DEM contact model. Nanoindentation is a useful technique that coupled with DEM simulations contributes to get a deeper look into the mechanical properties of the electrodes. Ultimately, this study provides a comprehensive understanding of how the interaction among the electrode components may affect the mechanical and electrochemical properties of the whole structure, which is of great relevance for designing high-quality electrodes to fulfil aimed specific requirements.