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► **To cite this version:**

Théo Boivin, Benoit Mathieu, Olivier Gillia, Willy Porcher. On the mechanical discrete approach of silicon/graphite-based anode breathing. ModVal 2023 - 19th Symposium on Fuel Cell and Battery Modeling and Experimental Validation, Mar 2023, Duisburg, Germany. , 2023. cea-04048256

HAL Id: cea-04048256

<https://cea.hal.science/cea-04048256>

Submitted on 27 Mar 2023

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On the Mechanical Discrete Approach of Silicon/Graphite-based Anode Breathing

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In the current researches intended to improve the Lithium-ion batteries capacity for automotive or electronic devices applications, enriching anode with silicon is one of the forehead solutions¹. However, silicon shows a tremendous volume change of +280% in the fully lithiated state², leading to a significant « breathing » of electrodes during cycling. When combined with more or less rigid casings, detrimental pressure or deformation levels can be reached and raise safety and performance issues. Hence, prediction of the volume changes related to applied pressure is key to design the cells. Irreversible volume changes are observed and conjectured to be related to microstructure changes², but current publications addressing the modelling aspects mostly use analytical or continuous models that can hardly capture the nonlinear changes of granular media microstructure. In that sense, *Discrete Elements Methods* (DEM) has proven to efficiently simulate granular medias³. Thus, this study aims to apply DEM on a silicon-based anode in order to take into account the discrete microstructure in the breathing behaviour.

The core of this work is to use the DEM software LIGGGHTS[®] on a sample of anode, modelled as a 3D distribution of spherical particles that can mechanically interact with each other. The breathing amount during charge and discharge cycles is evaluated via evolutions of thickness, void volume, porosity and coordination number. The global approach follows a progressive enrichment of contact laws, and successive sensitivity analysis of each upgraded parameter evaluate their capacity to reproduce more finely the observed behaviours. Besides, a systematic statistical analysis of initial random particles distribution is lead in order to avoid false interpretation of some evolutions.

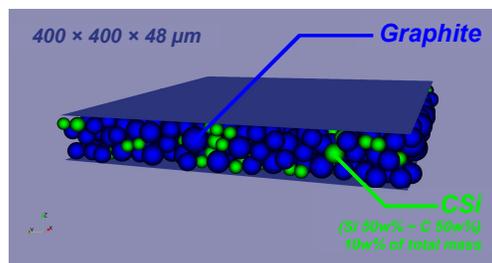


Figure 1 : DEM model of anode sample

In the parameters studied so far with the model, the coefficient of friction between particles, the confinement pressure applied on the anode and the adhesion are three major parameters that affect the breathing of the anode. Indeed, considering the change of anode thickness, the coefficient of friction analysed from 0.005 to 0.6 increases the breathing range with a factor of 1.5, the pressure analysed from 0.01 to 100 MPa decreases the breathing range with a factor of 1.7. Moreover, the adhesion analysed from 0 to 100 J/m² is able to create an irreversibility at first cycle of around 30% of breathing range which reproduce a characteristic experimental observation.

As a result, DEM showed its potential to introduce the granular properties in the anode model and explain some phenomena of irreversibility. It is a useful tool to determine the physical parameters to focus on, with a view to increase the reliability of the batteries. More parameters are planned to be explored, such as inter-particles bonds, plasticity and non-spherical particles. An experimental macroscopic measurements using a controlled-pressure test bench will be carried out to complete the available data².

Keywords: Lithium-ion battery, anode, breathing, Discrete Element Method, DEM, silicon-graphite

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