Influence of coprecipitation condition of $Ni_xMn_yCo_z(OH)_2$, used as precursor in ion lithium batteries cathodes

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Lithium ion batteries are widely spread in a great variety of devices. Metal lithium oxides are some of the traditional cathodes (eg $LiCoO_2$) as they are easy to prepare and have good performance. Recently, new cathode compositions have been developed, such as Li $Li(Ni_xMn_yCo_z)O_2$ (x + y + z = 1) since it has advantages because it reduces the high costs and toxicity associated with cobalt, and has a good balance between capacity, cyclability and thermal stability.[1] These cathodes can be obtained by calcining the precursor $Ni_xMn_yCo_z(OH)_2$ (NMC hydroxide) with LiOH. An economical and scalable method for synthesizing NMC hydroxide is by coprecipitation of transition metals with a complexing agent in basic medium. There is limited experimental data on this coprecipitation process and its influence on the characteristics primary particles obtained, such as their size distribution (PSD), surface area and porosity. Likewise, there are few computational models that provide a predictive tool to determine the characteristics mentioned and to understand the influence of mixing on particle coprecipitation.

In this work, we propose a systematic study of the influence of synthesis conditions in coprecipitation, to later validate a new computational framework that allows predicting the coprecipitation of NMC hydroxides. Finally, study the relationship between the characteristics of the hydroxide obtained as morphology, tap density, PSD and the electrochemical behaviour of the oxide obtained from this NMC hydroxide.

The NMC hydroxides were synthesized through a coprecipitation process that was carried out within a microscale vortex reactor with four inlets, for the entrance of the solutions into the mixing chamber. All experiments were performed under N_2 atmosphere, changing the proportions of Ni Mn and Co, and flow rates. The resulting particles were characterized to determine tap density, PSD and morphology, using DLS and SEM. Finally, the $Li(Ni_xMn_yCo_z)O_2$ obtained from the NMC hydroxide was used as a cathode and electrochemically characterized, analyzing its specific capacity and cyclability, in coin cells.

The research reported in this paper was funded by European Union, Horizon 2020 Programme, SimDome Project, Grant Agreement No 814492. The views and opinions expressed in this publication are the sole responsibility of the author(s) and do not necessarily reflect the views of the European Commission/Research Executive Agency.

Referencias

[1] Eom, J., Kim, M. G., & Cho, Journal of The Electrochemical Society, 155 (3) (2008), A239-A245.