World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:11, No:05, 2017

Li2S Nanoparticles Impact on the First Charge of Li-ion/Sulfur Batteries: An Operando XAS/XES Coupled With XRD Analysis

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Abstract : With their high theoretical energy density (~2600 Wh.kg-1), lithium/sulfur (Li/S) batteries are highly promising, but these systems are still poorly understood due to the complex mechanisms/equilibria involved. Replacing S8 by Li2S as the active material allows the use of safer negative electrodes, like silicon, instead of lithium metal. S8 and Li2S have different conductivity and solubility properties, resulting in a profoundly changed activation process during the first cycle. Particularly, during the first charge a high polarization and a lack of reproducibility between tests are observed. Differences observed between raw Li2S material (micron-sized) and that electrochemically produced in a battery (nano-sized) may indicate that the electrochemical process depends on the particle size. Then the major focus of the presented work is to deepen the understanding of the Li2S material charge mechanism, and more precisely to characterize the effect of the initial Li2S particle size both on the mechanism and the electrode preparation process. To do so, Li2S nanoparticles were synthetized according to two ways: a liquid path synthesis and a dissolution in ethanol, allowing Li2S nanoparticles/carbon composites to be made. Preliminary chemical and electrochemical tests show that starting with Li2S nanoparticles could effectively suppress the high initial polarization but also influence the electrode slurry preparation. Indeed, it has been shown that classical formulation process - a slurry composed of Polyvinylidone Fluoride polymer dissolved in N-methyle-2-pyrrolidone - cannot be used with Li2S nanoparticles. This reveals a complete different Li2S material behavior regarding polymers and organic solvents when going at the nanometric scale. Then the coupling between two operando characterizations such as X-Ray Diffraction (XRD) and X-Ray Absorption and Emission Spectroscopy (XAS/XES) have been carried out in order to interpret the poorly understood first charge. This study discloses that initial particle size of the active material has a great impact on the working mechanism and particularly on the different equilibria involved during the first charge of the Li2S based Li-ion batteries. These results explain the electrochemical differences and particularly the polarization differences observed during the first charge between micrometric and nanometric Li2S-based electrodes. Finally, this work could lead to a better active material design and so to more efficient Li2S-based batteries.

Keywords : Li-ion/Sulfur batteries, Li2S nanoparticles effect, Operando characterizations, working mechanism
Conference Title : ICEMT 2017 : International Conference on Electrochemical Materials and Technology
Conference Location : Rome, Italy
Conference Dates : May 04-05, 2017