Materials Panel Abstract & Speaker Biography

Li2S particle size influence on the first charge working mechanism of Li2S based Li-ion batteries analysed by operando X-ray absorption and emission spectroscopies coupled with operando X-ray diffraction

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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 S_8 by Li_2S as the active material allows the use of safer negative electrodes, like silicon, instead of lithium metal. S_8 and Li_2S 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 [1] (Figure 1a). Differences observed between raw Li_2S material (micron-sized) and that electrochemically produced in a battery (nano-sized) may indicate that the electrochemical process depends on the particle size [2].

Then the major focus of the presented work is to deepen the understanding of the Li_2S material charge mechanism, and more precisely to characterize the effect of the initial Li_2S particle size both on the mechanism and the electrode preparation process. To do so, Li_2S nanoparticles were synthetized according to two ways: a liquid path synthesis [3] and a dissolution in ethanol, allowing Li_2S nanoparticles/carbon composites to be made [4]. Preliminary chemical and electrochemical tests show that starting with Li_2S nanoparticles could effectively suppress the high initial polarization (Figure 1b) 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 Li_2S nanoparticles. This reveals a complete different Li_2S 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. The results allow us to explain the electrochemical behavior and particularly the polarization differences observed during the first charge between micrometric and nanometric Li_2S-based electrodes. Finally, this work could lead to a better active material design and so to more efficient Li_2S-based batteries.

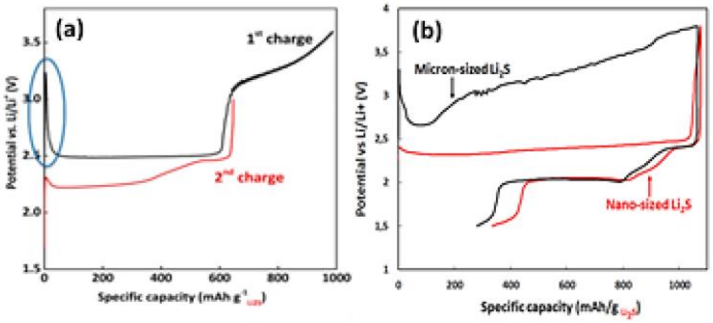

Figure 1: *(a) Typical voltage profiles of two first charges of a Li_2S-based cell* [1] *and (b) comparison of voltage profiles between micro and nano-sized Li_2S particles-based cell.*

References

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Speaker Biography:

After being graduated in electrochemistry at the Engineer School PHELMA in 2014, Alice Robba is currently preparing her PhD degree on the development of Li-ion/Sulfur batteries. Her PhD studies are carried out between two laboratories in Grenoble: the Electrochemistry and Physicochemistry of Materials and Interfaces Laboratory (LEPMI) and the CEA-Liten.

Her work mainly focuses on the development of positive electrodes in the Li-ion/Sulfur batteries by analyzing the impact of the active material (Li_2S) microstructure on the electrochemical performances. She also works on the working mechanism and particularly on the poorly understood first charge of the Li-ion/Sulfur batteries.