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Investigations of the solid-electrolyte interface in an all-solid-state battery using ToF-SIMS

All solid-state batteries are a rapidly expanding field with complex formations of both the anode and cathode materials. Solid-state lithium sulfur batteries provide increased energy storage and improved safety. We investigate the composition and formation of the solid electrolyte interface (SEI) for pristine and cycled sulfur-based solid-state batteries. We compare two sulfide solid state electrolyte, namely, Li_6PS_5Cl (LPSCL) and $Li_{10}GeP_2S_{12}$ (LGPS). The cathode material composition is LiNi0.8Mn0.1Co0.1 O2 (NMC811). These nickel rich layered oxides provide contributions to energy storage and act as the active material offering high capacitance and voltage while the sulfide solid state electrolyte offers increased ionic conductivity. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) was used to acquire surface spectra, depth profiles, 2D secondary electron (SE) images, and secondary ion 2D/3D images of the SEI. SIMS spectra and images were gathered using the 30 keV Bi3+ primary ion beam over a 500 × 500 μm2 area for 60 scans. Depth profiles were obtained using the 2 keV Cs+ sputter beam and 30 keV Bi3+ primary ion beam over a 100 × 100 μm2 area for 250 scans. Sulfur clusters (Sx) were observed, which were attributed to the deformation of the cathode surface after cycling. The mass spectral analysis and 2D/3D results imaged the SEI with formation of sulfates, phosphates and fluorine compounds. Comparisons of the LPSCL and LGPS in spectral analysis and 2D/3D imaging illustrate that LPSCL has higher counts of SEI formation products as well as indication of bubbling on the surface. In contrast, LGPS has pitting. Our results show that ToF-SIMS can uncover the mechanistic differences in SEI formation of all solid-state batteries.

Topical Area

Hard matter: energy materials

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