

One-step synthesis of amorphous MoO_xS_y as a high-performance anode material for Na-ion batteries

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Recently, conversion reaction based electrode materials such as transition metal (TM) oxide, sulfide, and phosphide, which have mostly been studied as high-capacity electrodes for Li-ion batteries (LIBs), have been investigated for possible high-capacity Na-ion batteries (NIBs) anodes. Similar to conversion reaction with Li, all possible valance states of transition metals (TMs) in the materials can be utilized, enabling more than one electron redox reaction per TM, which leads to a generally high specific capacity. However, poor conductivity which cause large hysteresis and low reversibility and huge volume change during sodiation/desodiation which deteriorate cycling stability plague many conversion reaction.

Over the past decade, nanostructured materials have been widely used to enhance these problem of conversion reaction based electrodes by shortening both electronic and ionic pathway and relieving stress during sodiation/desodiation. However, fabricating nanostructured materials usually involves multiple complicated steps, and large surface area of the nanostructure accelerates electrolyte decomposition which induces large irreversible capacity and contact loss between electrode material and current collector upon repeated cycling.

There have been several reports showing that the intrinsically isotropic nature in amorphous materials, which can mitigate the large volume changes associated with charge/discharge process, improve the cycling stability of rechargeable batteries. In addition, amorphous materials are also advantageous in terms of Na-ion diffusion, which might be facilitated by the presence of percolation pathways. Based on the above issues, faster reaction kinetics, better reversibility and narrower voltage hysteresis would be anticipated for amorphous anode. However, little is known about the microscopic mechanisms involved in the reaction of amorphous electrodes, such as the nucleation and evolution of the metal phases and their phase distribution on the nanoscale.

Herein, we propose to design a bulk-type amorphous MoO_xS_y anode for Na-ion batteries using an ultra-simple and facile electrodeposition process. In this study, as well as electrochemical performance measurements, we investigated the structure and phase evolution of the a- MoO_xS_y during first sodiation and desodiation to better understand the mechanisms underlying the conversion process and the electrochemical behavior. High-resolution transmission electron microscopy (TEM), which was often used to characterize the structure of the converted phases, provides sufficient contrast only for a fraction of the metallic particles; little contrast is observed for the Na_2S or Na_2O due to the weak scattering of the light constituent elements. In addition, X-ray absorption fine structure (XAFS) measurements, sensitive to short-range order, were used to track the structure and phase evolution of the electrodes during the conversion process.