Computational study on the mechanical stability of novel Sn/C composite particulate structure as potential anodes for rechargeable Na ion battery

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The global demand for electrical energy storage (EES) devices for efficient energy storage, grid scale applications and delivery purposes is increasing at an alarming rate. Chemical storage technologies based on rechargeable batteries are considered as one of the leading and promising technologies for EES. Since its introduction and commercialization by Sony in 1991, Li ion batteries are preferred rechargeable battery systems for portable electronic devices. However, in the past few years, Na ion based secondary battery technologies are also witnessing significant interest and attention [1]. Sodium is relatively cheaper and more abundant in the earth's crust compared to lithium. Na ion battery is also potentially easy to engineer and poses less safety issues, as it is chemically more stable and environmentally benign compared to the Li based battery system. Even though the research in Na ion secondary batteries is still in its developing stages, it is expected to emerge as a possible alternative to Li ion batteries.

Tin based anodes for Na based batteries have garnered attention due to its high theoretical capacity of ~847 mAh/g owing largely to the formation of $Na_{15}Sn_4$ zintl type alloy phase. However, the alloying reaction results in a large ~400% volumetric expansion. This colossal volumetric expansion can cause degradation of the Sn anode leading to loss of capacity. Experiments reported in the literature to date show that the electrochemical performance of the electrodes composed of micron size tin particles degrades rapidly. However, the performance is much improved if the anode particles have a matrix of carbon surrounding the Sn particles. Our recent experiments also show that the performance is significantly improved if the particle size is reduced from micron size to the nano scale[2].

We will present the results of our study conducted on the mechanical stability of Sn/C based anode system using a thermodynamically consistent theoretical framework. The transport of Li is coupled with the mechanical stress field in a finite deformation setting. Diffusivity of Na inside Sn derived from experiments (GITT and CV) will be utilized in this model. The framework is employed in a finite element based computational model to simulate the coupled phenomena [3]. We will discuss the effect of Sn particle size on the stress generation inside the electrode. We will also evaluate the alleviating effect of C matrix on the electrode mechanical stability. We will demonstrate that Sn particles undergo plastic deformation depending on the size of the particle and the degradation affects the the constitutive properties of Sn as well as the matrix. This damage tends to accumulate over consecutive electrochemical cycles thus affecting the overall electrochemical response.

Reference:

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