



# Chemomechanics of Advanced Energy Storage Materials

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We present our recent results in the analyses of chemomechanics in advanced energy storage materials: (a) Si nanomaterials/nanostructures for Li-ion battery anode applications. The theoretic capacity of the state-of-the-art Li-ion batteries with graphite-based anodes is limited to 372 mAh/g. In comparison, Si anode has the theoretic capacity of 4200 mAh/g, over 10 times that of graphite-based anodes. However, silicon exhibits large volume expansion (~400 %) upon Li-ion insertion. The stress induced by this volume change causes cracking, pulverization and peeling off the underlying current collector, leading to loss of electrical contact and eventual fading of capacity. Here nanoengineering approaches will be discussed that can mitigate this effect by modulating the nanostructure and composition of the active material. It is followed by a rigorous chemomechanical formulation of the problem and some recent results. (b) Mg nanoblades for solid-state hydrogen storage. In a combined experimental and theoretical study, it was shown that the H-diffusion constant in  $MgH_x$  between Mg and  $MgH_2$  varies by nearly three orders of magnitude. The strong concentration dependence of H diffusion constant throws profound influence on the stability and instability of a diffusion front: an H diffusion front in hydrogenation, and an H-vacancy diffusion front in dehydrogenation. In the latter case, the front tends to corrugate forming islands of Mg hydride in the worst scenario. The predicted diffusion-induced stress and plastic deformation fields are highly non-uniform. It may precede severe morphological changes of Mg nanoblades and turn them into powder over cycling, consistent with the experimental observations.

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**Prof. Bo Yang** is an Assistant Professor of Mech. & Aero. Eng. at UT Arlington. He earned his BS from the University of Science and Technology of China in 1992, and his PhD from the University of Houston in 1998. Prior to joining UTA, he taught at Florida Institute of Technology in 2003-2011. His primary research interests are in micro/nanomechanics of defects and cracks, cell and tissue mechanics, fracture mechanics of composite materials, and computational methods. He has published > 40 journal articles and served as a peer reviewer for > 30 journals. He serves on the Editorial Board of *International Journal of Computers, Materials, & Continua*, and is a member of ASME and Materials Research Society.

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