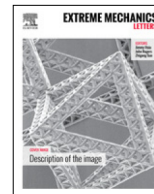




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Failure mechanics of a wrinkling thin film anode on a substrate under cyclic charging and discharging

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GRAPHICAL ABSTRACT



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ABSTRACT

Recent experiments show that a thin film anode on a compliant substrate can significantly mitigate mechanical degradation and capacity fading of lithium-ion and sodium-ion batteries in service. The enhanced cycle performance of such a substrate-supported thin film anode is attributed to the wrinkling-induced stress relaxation. While the experimental evidence is suggestive, there lacks a systematic mechanistic study of the wrinkling of the substrate-supported thin film anode and its influence on anode cycle performance. We report a comprehensive study of the charging/discharging induced wrinkling formation and subsequent morphologic evolution of a substrate-supported thin film anode, using theoretical analysis and finite element simulations. We reveal that necking bands may form near wrinkling troughs or peaks and further develop to cause fragmentation of the anode over charging/discharging cycles, a failure mode not reported in the existing literature. The density and distribution of the wrinkling-associated necking bands in the substrate-supported thin film anode can be regulated by the substrate stiffness. Moreover, the wrinkling-induced necking in such a thin film anode can be deferred by regulating the charging capacity. These findings offer new mechanistic understanding of substrate-supported thin film anodes and thus shed light on novel design of high performance anodes in batteries.

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1. Introduction

The past decade has seen a surge of interest in developing next-generation rechargeable batteries with high capacity and long cycling life with an array of diverse

applications ranging from portable electronics to electric vehicles, and to grid scale energy storage [1–7]. There exist intensive studies to search candidate electrodes with high electrochemical capacity and mechanical durability. For example, silicon (Si) has the highest theoretical capacity of 4200 mAh/g when fully lithiated in lithium-ion (Li-ion) batteries [8] and tin (Sn) alloys with sodium (Na) in Na-ion batteries at a capacity of 847 mAh/g when $\text{Na}_{15}\text{Sn}_4$

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is formed [9]. However, extreme volumetric expansion (e.g., 300%–400%) is often associated with the fully charged state of such electrode materials, which in turn causes anode pulverization and thus leads to rapid capacity fading and poor cycle performance of the batteries [10–15]. Therefore, averting the mechanical degradation of anodes induced by the extreme volumetric change during charging/discharging cycles remains as one of the major challenges in developing high performance Li-ion and Na-ion batteries.

Tremendous efforts have been focused on mitigating the mechanical failure of anodes in high-performance Li-ion and Na-ion batteries. Charging/discharging-induced stress and associated mechanical failure in Si and Sn anodes are widely studied through experimental characterization [16–19] and chemo-mechanical modeling [11,13,20–30]. As revealed from these studies, size reduction, geometry optimization and surface passivation of the anodes are shown to be able to mitigate excessive stresses induced during charging/discharging and thus help avoid pulverization of anodes [12,13,20,31]. For example, it has been demonstrated that nanoscale Si anodes, such as nanowires [32], nano-particles, nano-beads [31], nano-walls [33] and nano-sized thin films [34] exhibit superior cycle performance than their bulk counterparts [35], largely due to the reduced driving force for crack propagation in such anodes. Hollow Si nanowires and nanospheres are shown to not only relieve lithiation-induced stresses but also reduce the impeding effect of such stresses on lithiation kinetics [36]. Surface passivation of anodes using functional coatings such as carbon [37], nickel [38,39], silicon oxides [40,41] and aluminum oxides [9] can avoid the repeated formation of excess solid-electrolyte-interface (SEI) layers and mediate mechanical degradation of anodes such as fracture and detachment from current collector [42].

It has been shown that a thin film can be made deformable by leveraging out-of-the-plane buckling and wrinkling to accommodate large in-plane deformation without resulting in significant strain in the film material [43,44]. Such a concept has been successfully used in designing highly deformable flexible electronic devices [45–47], and recently been applied to design durable anode structures that can sustain the huge deformation associated with charging/discharging. For example, Bhandakkar et al. computationally demonstrate that honeycomb-shaped anodes allow for buckling deformation mode during lithiation and delithiation, which effectively reduces the resulting stresses [48]. Yu et al. reported that Polydimethylsiloxane (PDMS)-supported thin ribbon Si anodes can yield a cycle performance up to 500 cycles with nearly 85% capacity retention [34], which is attributed to the mitigation of lithiation-induced stresses via wrinkling of the Si ribbons. Zhu et al. showed that an anode for Na-ion battery consisting of a thin Sn film bonded to a soft wood fiber substrate can sustain more than 400 charging/discharging cycles, while a similar thin film Sn anode on a rigid substrate suffers from severe capacity decay after only 10 s cycles [9]. Chemomechanical modeling reveals that the wrinkling of the Sn film during sodiation/desodiation leads to effective stress relaxation, a key

to the enhanced mechanical integrity and electrochemical performance of the anode.

While the experimental evidence of leveraging wrinkling for designing durable anodes is suggestive, there lacks a systematic mechanistic study of the wrinkling of substrate-supported thin film anodes and its influence on anode cycle performance. Some fundamental but crucial questions remain elusive so far. For instance, while it is shown that wrinkling can lead to stress relaxation in thin film anodes, it remains unclear what is the fundamental deformation mechanism that governs the mechanical failure of such wrinkling thin film anodes under cyclic charging/discharging. Furthermore, existing computational studies of the wrinkling thin film anodes are conducted for only the first charging/discharging cycle. How does the wrinkling morphology of the thin film anode evolve over cycles and how does such an evolution of wrinkling morphology subsequently affect the battery performance? Aiming to address these open questions, in this paper, we report a comprehensive study of the charging/discharging induced wrinkling formation and subsequent morphologic evolution of a substrate-supported thin film anode, using both theoretical analysis and finite element simulations.

Emerging from the present comprehensive study is a failure mechanism of a thin film anode supported by a compliant substrate subject to electrochemical charging/discharging cycles that is distinct from that of a thin film anode supported by a stiff substrate. Fig. 1 summarizes the difference in the failure mechanisms of these two anode architectures. During the first charging half cycle, the thin film anode thickens to accommodate the volume increase due to ion insertion. The substrate constraint further increases the compressive stress in the thin film anode. Well bonded to a stiff substrate, the thin film anode remains planar during the charging half cycle. By contrast, on a compliant substrate, the thin film anode starts to wrinkle, driven by the charging-induced compressive stress and accommodated by the substrate distortion. As to be shown later, the wrinkling occurs in a rather periodic manner with a wavelength λ_w that is governed by the anode thickness and the anode/substrate stiffness ratio. During the first discharging half cycle, ion extraction causes the thinning of the anode. Consequently, on a stiff substrate, substantial tensile stress builds up in the thin film anode so that channel cracks may initiate and propagate in the anode in a rather random fashion. By contrast, during the first discharging half cycle, the wrinkled thin film anode on a compliant substrate thins and flattens simultaneously, accompanied by a peculiar feature of necking formation in the thin film anode near the troughs or peaks of the wrinkling morphology. In subsequent charging/discharging cycles, the above morphological evolution of the thin film anode continues, leading to two distinct mechanical failure modes of the two anode architectures. For a thin film anode bonded to a stiff substrate, more and more channel cracks form and propagate in the anode in a random fashion, eventually causing the pulverization of the anode, as observed in many experiments [49,50]. By contrast, for a thin film anode bonded to a compliant substrate, the wrinkling

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