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Understanding the role of mechanics in energy materials: A perspective

Kejie Zhao [a,*], Yi Cui [b,c,*]

[a] School of Mechanical Engineering, Purdue University, West Lafayette, IN 47906, USA
[b] Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, USA
[c] Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA

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1. Overview

Mechanical issues are ubiquitous in energy storage, conversion, and harvesting. Cracks occur in solid oxide fuel cells due to the thermal stresses and non-stoichiometry of oxygen in the electrodes and electrolyte [1,2]. In photovoltaics, the low resistance to cohesive fracture of perovskite films deteriorates the structural reliability and inhibits the success of perovskite solar cells as a viable technology [3]. In capacitors using ferroelectric thin films, the mismatch strain caused by the electric polarization leads to the presence of a disruptive dead layer at the metal–dielectric interface and a capacitance drop [4,5]. In hydrogen storage, the interplay between hydrogen and localized plasticity of the fuel containers causes embrittlement [6]. In batteries, mechanical degradation compromises the capacity in current technologies and becomes a limiting factor for the implementation of high-energy-density electrodes [7]. Conversion of mechanical energy to electricity through piezoelectric and triboelectric effects has also attracted recent interests [8,9].

There have been rapid advances in theories, modeling, and experimental characterizations of mechanical behaviors of advanced energy materials and systems over the past few years. The phenomenal progress highlights the significance of mechanics perspectives on the energy solutions. Meanwhile, the field of strongly coupled physicochemical processes and mechanics provides a platform to advance the frontier of fundamental mechanics. The themed issue on Mechanics in Energy Materials aims to feature the-state-of-the-art of mechanics in the interdisciplinary field of energy materials.

The special issue has an excellent collection of eighteen articles highlighting the critical role of mechanics in various forms of energy materials. In photovoltaic solar cells, Rolston et al. highlight the issue of mechanical integration of solution-processed perovskite solar cells [3]. They measure the fracture resistance of a multitude of solution-processed organometal trihalide perovskite films and cells and determine the influence of stoichiometry, precursor chemistry, deposition techniques, and processing conditions on the fracture resistance of perovskite layers. Lin et al. present an exciting photoluminescence technique to identify and categorize dislocation defects near the low/high angle grain boundaries [10]. The technology may form the basis of full field optomechanics characterization of materials for solar energy conversion. In batteries, both the cathodes and anodes have outstanding mechanical issues. McDowell, Xia, and Zhu provide an overview of mechanics of large-volume-change transformations in high-capacity battery materials, and highlight the synergistic in situ observation of real-time reactions and

* Corresponding authors.
E-mail addresses: kjzhao@purdue.edu (K. Zhao), yicui@stanford.edu (Y. Cui).

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mechanical degradation processes, measurements of mechanical properties, and experiments and simulations of spatiotemporal stress generation and evolution in active materials and structures across various length scales [11]. Kim et al. present a high throughput combinatorial analysis of mechanical and electro-chemical properties of $LiNi_xCo_yMn_zO_2$ cathode using gradient deposition thin film electrodes and nanoindentation [12]. A strong correlation between the enhanced electrochemical performance and retention of mechanical properties of electrodes is shown. For the composite electrodes of microscopic heterogeneity, Vasconcelos et al. use grid indentation and statistically analysis to determine the mechanical properties of active and inactive materials as well as the inter-phases [13]. The wafer curvature method is the state-of-the-start technique to determine the stress evolution in thin film electrodes during the charge and discharge cycles. Tokranov and Sheldon utilize this measurement to investigate the stresses induced by propylene carbonate (PC) additions to a standard liquid electrolyte [14]. They show that the PC additions lead to a very low value of the interlaminar fracture resistance. Nicholas provides a detailed discussion on practical considerations for the measurement of stresses and oxygen surface exchange coefficients from the bilayer curvature relaxation method [15]. Barai et al. consider the poromechanical effect in the Li–S battery cathode and build a computational methodology to quantify the impact of precipitation induced volume change, pore morphology, and confinement attributes in a Li–S cathode [16]. Sun et al. study the fragmentation of active material secondary particles in Li-ion battery cathodes induced by lithiation cycles using combined analytical and numerical modeling [17]. Zuo and Zhao develop a phase field model that couples Li diffusion, finite deformation, stress evolution, and crack propagation and considers the effect of elastic softening and plastic flow [18]. Wang et al. model the inelastic shape changes of Si particles and stress evolution at the binder/particle interface in a composite electrode during lithiation/delithiation cycles [19]. Wang and Chew use large-scale molecular dynamic simulations to elaborate the atomistic mechanism of elastic softening and plastic flow of lithiated Si [20]. Wang et al. report an experimental approach to monitor the real-time temperature evolution of coin cells [21]. In the application of electric vehicles, Kukreja et al. propose a multifunctional, damage tolerant battery system which combines the energetic material with mechanically sacrificing elements that control the mechanical stresses and dissipate energy [22]. In addition to the themed articles on batteries and solar cells, Jin et al. synthesize crystalline P-type $Bi_xSb_{2-x}Te_3$ nanowires using pulsed laser assisted electrochemical deposition to enhance the thermoelectric performance [23]. Yu and Wang review recent processes of chemical modifications of triboelectric polymers for the emerging technology of triboelectric nanogenerator [24]. Nian et al. utilize additive roll-to-roll printing to produce cold welding of 2D crystal and 1D nanowire layers for flexible transparent conductor and planer energy storage [25]. Zhai et al. systematically investigate the influence of surface topology on interfacial electro-mechanical properties, including contact stiffness and electrical conductance at rough surfaces under varying compressive stresses, for the multiple components in energy systems [26].

The special issue is a timely contribution to emerging field of electro-chemo-mechanics in energy conversion/storage. With the opportunity of overviewing the themed articles in the special issue, we, as the guest editors, would like to provide a short perspective in understanding the role of mechanics in the interrelated processes of energy materials. The Cui group at Stanford University studies fundamentals of nanomaterials including nanowires, colloidal nanocrystals, and patterned nanostructures, and develop low-cost processes in energy conversion and storage, electronics, biotechnology, and environmental technology. The Zhao group at Purdue University is focused on characterizing the chemomechanical behaviors of energy materials using in-situ experimentation and multiscale modeling. We will use Li-ion batteries as a vehicle to elaborate the mechanical issues in the current technology of batteries and future implementation of high-capacity electrodes, the fundamental coupling of mechanics with the thermodynamics and kinetics of electrochemical reactions, and use of mechanics principles to design mechanically resilient electrode materials and structures.

2. Mechanical failure in Li-ion batteries

Batteries occupy a privileged position in energy storage. The total size of the battery market accounts for $54 billion (US) in 2013 and a 5% growth rate per year is projected between 1990 and 2013 [7]. Li-ion batteries are a key enabler for portable electronics and electrification of automotive transportation. The global market by 2020 is estimated to be $32 billion for Li-ion technology alone. Reliability of batteries is crucial *per se* in such large-scale applications and has a direct impact on the societal economics.

Mechanical failure in Li-ion batteries is significant, as highlighted in a recent review article in *Science* [7]. The stress-induced structural disintegrity impedes electron conduction and increases the electric and ohmic resistances. Furthermore, mechanical deformation of the active material interferes with the stability of solid electrolyte interface (SEI) which results in a persistent decrease of cyclic efficiency. Fig. 1(a) shows a brief survey of the volumetric strains in the state-of-the-art cathode and anode materials for Li-ion batteries. Drastic deformation is inherent to the high-capacity electrodes, which places a grand challenge in the development of conversion- and insertion-type electrodes. Meanwhile, it is worth pointing out that mechanical failure is not only a unique issue in high-capacity materials, but also commonly occurs in the electrodes of relatively small volumetric deformation ($<10\%$). Fig. 1(b) exemplifies various sources of mechanical degradation including fracture of active particles, crack of inactive conductive matrix, crack and debonding of thin films, breakage of SEI, cavitation, and disintegration of particles in both anode and cathode materials which experience volumetric strains ranging from a few percentage to a few hundred percentage.

3. Fundamental coupling of mechanics with thermodynamics and kinetics of electrochemical reactions

From the mechanics perspective, Li-ion batteries provide an excellent example to study the intimate coupling between mechanics and electrochemistry [33]. The electrochemical process of Li insertion and extraction induces such rich phenomena of elemental mechanics as large elasto-plastic deformation [34], cavitation [35], reactive plasticity [36], and corrosive fracture [37]. Meanwhile, mechanical stresses modulate the thermodynamics and kinetics of ionic transport, surface charge transfer, interfacial reaction, and phase transition of materials [38]. The mechanical degradation of batteries is now recognized, maybe less understood is the influences of stresses on the electrochemical reactions. A conventional wisdom, for a system involving multi-physical processes, is that "chemistry always win" simply because the energy scales in the chemical reactions are usually orders of magnitude higher than the mechanical energies [39]. Li-ion batteries might be an exception from this rule in that the chemical driving force (bonding energy) in the lithiation/delithiation reactions is relatively weak in order to maintain a good cyclability [40], while the mechanical deformation and stresses are often significant that leverages the mechanical energy to a level comparable with the

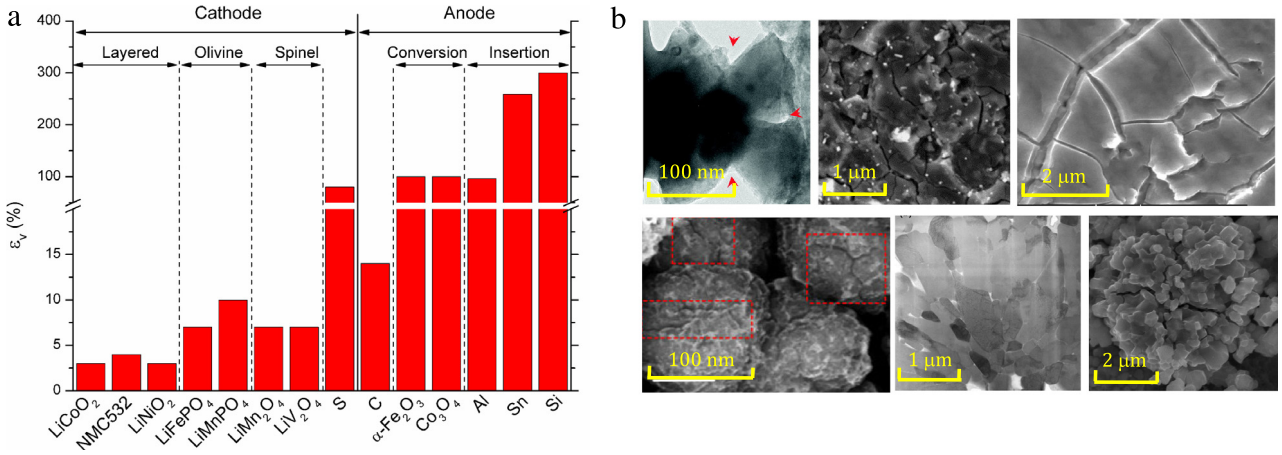

Fig. 1. (a) Volumetric strains upon lithiation [27]. (b) Various forms of mechanical degradation including fracture of Si particles [28], crack in C conductive matrix [29], debonding of Si thin films [30], breakage of SEI in Co_3O_4 particles [31], cavitation in NMC622 [32], and particle disintegration in NMC532.

chemical energies. The advance of electro-chemo-mechanics in Li-ion batteries may provide an opportunity to branch the frontier of applied mechanics.

Fig. 2 sketches a few theories and observations that originate from the coupling of electrochemistry and mechanics, including diffusion-induced stresses, stress regulated surface charge transfer, interfacial reaction, inhomogeneous growth of lithiated phases, instability of solid-state reaction front (SSRF), as well as reaction-assisted plastic flow and corrosive fracture. Many of the phenomena are at early stage of study and are to be further explored. Fig. 2(a) shows the diffusion–stress coupling—diffusion of Li atoms generates a field of stress, and the local stresses affect the chemical potential of Li, whose gradient tends to homogenize the distribution of Li. For a free-standing spherical particle with a given Li flux prescribed at the outer shell, the shell region (Li rich) is under compression and the core region (Li poor) is under tension. Stress modifies the chemical potential of Li and drives Li migrate from the compressed part to the tensed core. Fig. 2(b) demonstrates the free energy diagram altered by the applied electrical potential and mechanical stresses. The activation energies of the redox reactions at equilibrium states are identical, $\Delta G_{00} = \Delta G_{0R}$, (black solid lines). The chemical equilibrium will be broken by the electrical overpotential $E - E_0$ as well as the mechanical stress, where E represents the electrical field and E_0 the equilibrium potential. The electrical overpotential promotes electron transfer and decreases the free energy of the oxidized state by $F(E - E_0)$ (red dashed line). The tensile stress in the surface layer, on the other hand, causes a change of elastic energy $\Delta W = \sigma_m \Omega$ (blue dashed line) that promotes the formation of neutral Li, where Ω represents the partial molar volume of Li in the host, and σ_m is the mean stress. The change in the total free energy of the reduced state relative to the oxidized state is $F(E - E_0) - \sigma_m \Omega$. A modified Butler–Volmer equation can be introduced to include the stress effect [45]. In a recent work, Kim et al. made an ingenious use of the principle of stress-driven diffusion to design a novel class of mechanical energy harvesters [41]. The experimental setup is schematically shown in Fig. 2(c). Two identical partially lithiated Si films serve as electrodes separated by electrolyte-soaked polymer membranes. Bending-induced asymmetric stresses generate chemical potential difference, driving Li ions migrate from the compressed electrode (red) to the tensed side (blue) to generate electrical current. By removing the bending stress ion flux and electrical concurrent are reversed. The device can sustain more than a thousand cycles with nearly constant current output. The output electric current is determined by the concurrent surface charge transfer and Li bulk diffusion in the electrodes—both processes are dependent on the bending stresses as shown in Fig. 2(a) and (b). Fig. 2(d) illustrates the coupling between reaction and plasticity—when a host material is subjected to concurrent Li reactions and mechanical load, the valence state of matter is under dynamic change. The chemical reactions will promote plastic flow by decreasing the stresses needed to maintain a given atomic shear displacement [36]. Fig. 2(e) shows the schematic of concurrent Li diffusion and accumulation, Li weakening of the material strength, and crack propagation. Li is like a corrosive species. Li insertion breaks the host atomic bonds and forms weaker bonds between Li and host atoms, decreasing both elastic modulus and fracture strength of the host material. The dynamics of crack propagation is coupled with the kinetics of Li transport [37]. Li diffuse quickly on the crack surface because of the high surface diffusivity, and is accumulated at the crack tip due to the large tensile stresses ahead of the crack. Aggregated Li reduces the fracture toughness of the host material, acting as a corrosive agent that accelerates crack nucleation and propagation. The most dramatic effect of stress on electrochemical reactions may be the stress-induced stagnation of reaction front during lithiation of Si spherical particles [42]. The propagation of the reaction front induces a hydrostatic pressure in the crystalline core, which diminishes the thermodynamic driving force of lithiation and retards the electrochemical reaction, Fig. 2(f). For the system with interfacial reaction controlled kinetics, the stress field will be modified by the geometric factor of surface curvature. Fig. 2(g) shows the schematics of a structure with perturbed surface of small amplitude. It grows into a wavy morphology during lithiation reactions [43]. The formation rate of the lithiated phase is modified by stresses. The lithiated phase of convex curvature develops a field of tensile stresses, facilitating Li transport through the lithiated material and promoting the interfacial reaction at the phase boundary. On the contrary, a material element in the lithiated phase of concave curvature is under a field of compressive stresses, retarding the electrochemical growth. It is clear that the mechanical stress shapes the thermodynamics and kinetics of electrochemical reactions. One another interesting phenomenon is the instability of solid-state reaction front modulated by mechanical stresses. In an example nanowire, Fig. 2(h), lithiation induced stress breaks the planar solid-state reaction front into a curved interface and results in an uneven lithiation on a given basal plane [44], which may be a reminiscence of the Mullins–Sekerka interfacial instability during the solidification of a dilute binary solution [46].

4. Materials design to address the mechanical issues

The emerging nanotechnologies provide routes to enhance the chemomechanical stability of electrodes, and enable low-cost,

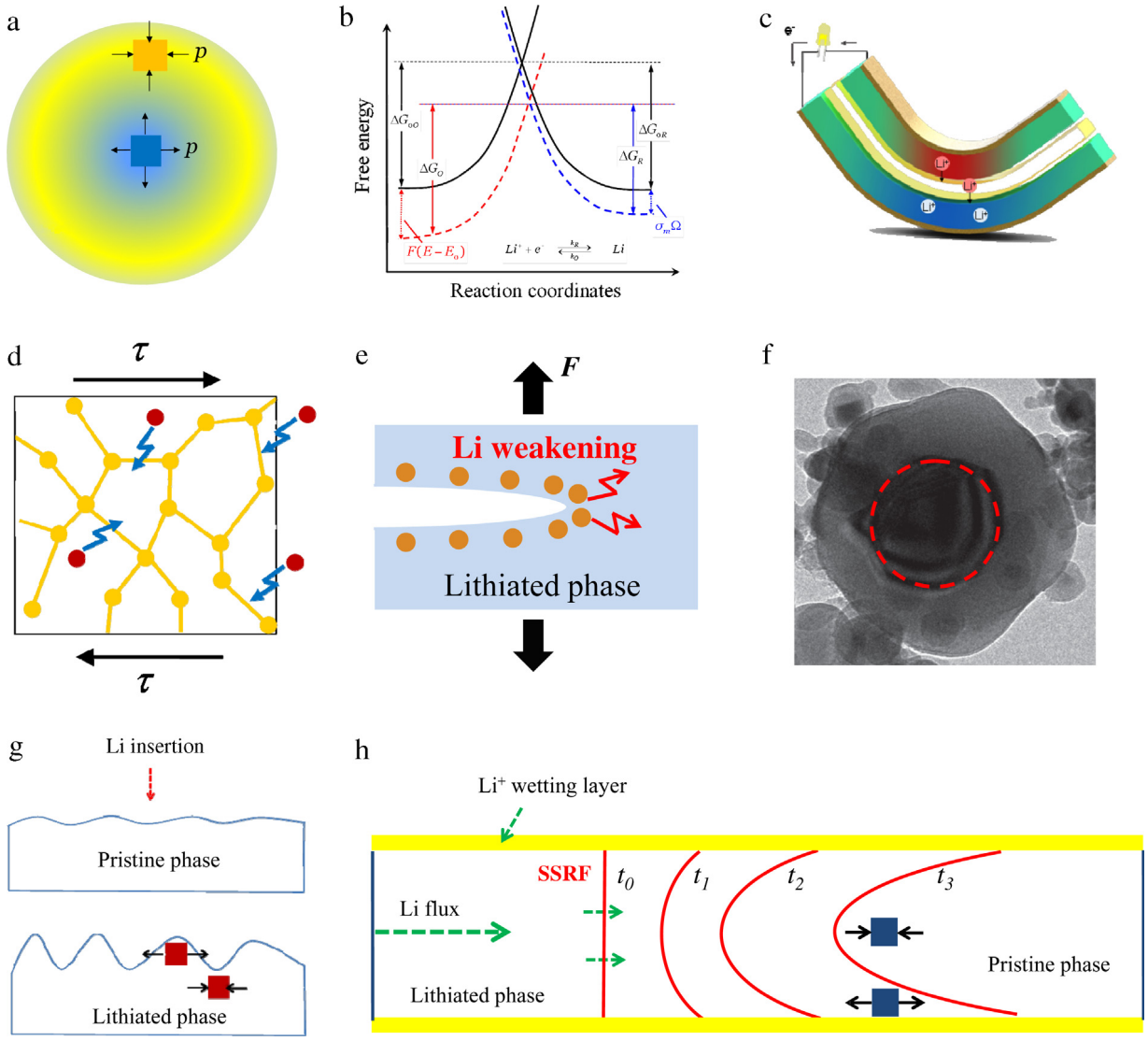

Fig. 2. Sketches of stresses coupled with the electrochemical processes. (a) Diffusion-induced stresses. (b) Stress-altered energy landscape of surface charge transfer. (c) Design of mechanical energy harvester based on the stress-driven Li diffusion [41]. (d) Coupled reaction and plasticity. (e) Corrosive fracture due to Li accumulation at the crack tip and weakening of the bond strength. (f) Stress-regulated interfacial reaction and stagnation of reaction front during lithiation of crystalline Si [42]. (g) Inhomogeneous growth of lithiated phase due to the curvature effect and stress regulated lithiation reaction [43]. (h) Instability of solid state reaction front modulated by stresses [44]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

fast fabrications of nanostructured materials with controls on the nanoscale size, shape, and chemical compositions. The small feature size enables flaw tolerance, accommodates the deformation, facilities ion transport, and promotes the rate capability by increasing the surface area of the electrodes to react with Li. Examples of nanostructures include nanowires, nanoparticles, core–shell structures, porous structures, and nanotubes [47–50], (Fig. 3(a)–(c)). Composite structures offers another paradigm to strengthen the performance of the electrodes. In a typical composite electrode, one material component contributes to the storage capacity of Li, while other functional elements, such as the conductive matrix, binders, or surface coating, provide the electric conductivity, mechanical support, or regulator for the electrochemical behaviors and mechanical deformation. A concept breakthrough to address the mechanical breaking issue due to large volume change yet maintaining a stable solid electrolyte interphase (SEI) is a confined hollow structure, which has a mechanically strong shell to confine the volume change towards interior hollow space. Such a confined hollow structure was first conceptually demonstrated in a double-walled hollow Si structure [51], (Fig. 3(d)), and was later extended to yolk–shell [52] (Fig. 3(e)) and pomegranate structures [53] (Fig. 3(f)). Another novel exciting material design strategy is to apply self-healing polymer to cure the breaks, which relies on non-covalent bonding to have the capability of repeatedly breaking and reforming [54] (Fig. 3(g)).

5. Conclusions

Mechanics is critical to a wide range of energy materials and technologies. When coupled with chemical, heat, and light, the mechanical stability often determines the reliability and durability of energy devices. The emerging field of electro-chemo-mechanics also offers a new platform to understand the role of mechanics in the intimately coupled physicochemical processes. Bridging the interdisciplinary fields of mechanics and materials science and electrochemistry with a focus of energy solutions can be truly rewarding for the fundamental science as well as technologies in large-scale applications.

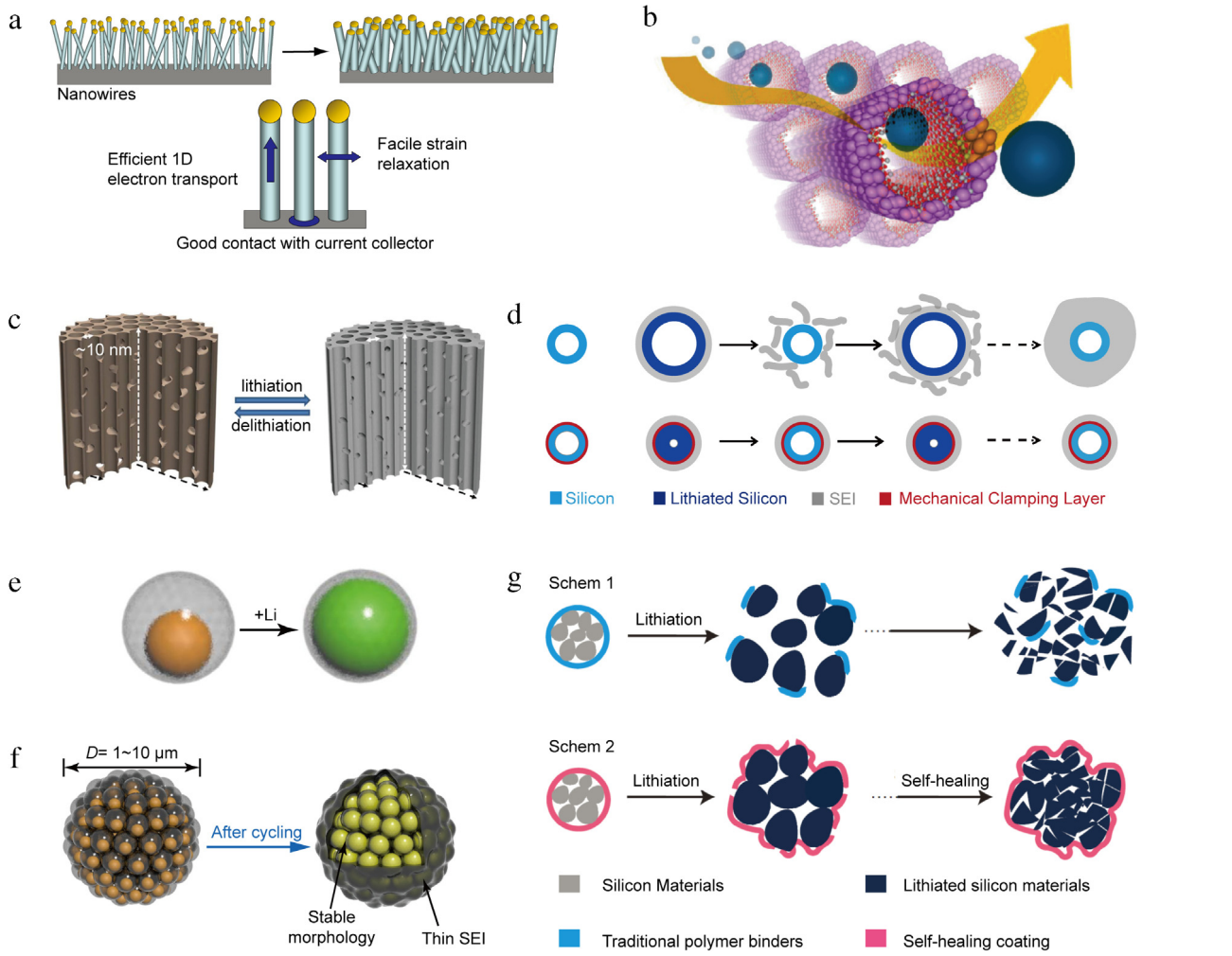

Fig. 3. Schematics showing the materials design to address the mechanical issues. (a) Si nanowires with good contact with current collector to avoid pulverization during cycling [47]. (b) Si nanotubes with hollow space to accommodate volume expansion [48]. (c) Si sponge with interconnected mesopores for tolerating volume expansion [49]. (d) Double-walled Si nanotubes with mechanically strong outer shells to prevent outward expansion and thus form stable SEI [51]. (e) A yolk–shell design that leaves void space within carbon shells to accommodate volume change [52]. (f) A pomegranate-like structure that significantly reduces the surface area and increases the packing density of nanostructures, which enables reduced side reactions and highly improved tap density [53]. (g) Schematic showing the self-healing polymer coating on the surface of Si microparticles, which can cure the breaks and guarantee good electrical contact with all wrapped Si even after pulverization [54].

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