



Self-healing strategy for Si nanoparticles towards practical application as anode materials for Li-ion batteries

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ABSTRACT

The overwhelming advantage of Si nanoparticles (SiNPs) over Si microsized particles (SiMPs) as anode materials is compromised by their severe side reactions with electrolyte and agglomeration during cycling. Unlike usual solutions such as surface encapsulation or coating, here, a new strategy was proposed by mimicking the self-healing ability of living organisms. Ureidopyrimidinone functionalized polyethylene glycol (UPy-PEG-UPy) was successfully synthesized. Taking it as binder, SiNPs achieved excellent electrochemical performance with an initial coulombic efficiency (ICE) as high as 81% and a reversible capacity of 1454 mAh/g after 400 cycles corresponding to an average capacity decay of 0.04% per cycle. This achievement is attributed to the self-healing ability of UPy-PEG-UPy, which enables to spontaneously heal micro-cracks on electrode prior to its propagation, therefore preventing Si particles agglomeration and maintaining electrode integrity.

1. Introduction

Owing to the highest known theoretical specific capacity, Si is recognized as the most promising anode material for high-energy-density lithium ion batteries (LIBs) [1–3]. However, its practical application is seriously impeded by poor cyclability and low initial coulombic efficiency as a result of mechanical and electrochemical instability, which mainly rooted in as high as 300% volume expansion of Si upon fully lithiation [4–7].

SiNPs have stronger mechanical tolerance to endure volume change than SiMPs, and therefore demonstrate better cycling performance [8–12]. However, severe side reactions with electrolyte due to large specific surface and agglomeration as a result of electrochemically driven sintering worsen its electrochemical performance [13–15] since the traditional binder is not capable enough to maintain Si electrode integrity upon cycling. It is therefore desired to develop novel binder to preserve SiNPs electrode integrity.

Inspired by self-healing ability of natural living organisms, artificial materials have been synthesized [16–18] with self-healing realized by external stimuli [19,20], which limits their application as binder. Through introducing a quadruple hydrogen bonding ureidopyrimidinone (UPy) moiety to polyethylene glycol (PEG) oligomers, in this work, UPy functionalized PEG with self-healing ability realized by no external stimuli was synthesized and investigated as

binder through comparison with a traditional binder poly(acrylic acid) (PAA).

2. Experimental

UPy-PEG-UPy was prepared by dissolving 6.1 mmol PEG, 3 drops of dibutyltindilaurate and 13 mmol 2(6-isocyanatohexylamino carbonylamino)-6-methyl-4[*IH*]pyrimidinone in 150 mL chloroform, refluxing the solution under an argon atmosphere, diluting with chloroform and ethanol, filtering over Celite, finally removing the solvent, subsequently, and then characterized by FTIR. Working electrode preparation and Swagelok-type three electrodes cell assembly were performed according to [21] except UPy-PEG-UPy binder was pre-dissolved into tetrachloroethane, and dried at 160 °C. SiNPs (50–70 nm), super C65 carbon black and UPy-PEG-UPy/PAA were in the weight ratio of 60:25:15 and 65:27:8, and the corresponding electrodes were denoted as UPy-PEG-Si-15 (8)/PAA-Si-15 (8), respectively. The electrolyte used was 1 M LiPF₆: EC + DMC (1/1 = v/v).

Galvanostatic cycling was performed in an Arbin BT2000 battery tester between 0.01 and 1.5 V. Electrochemical impedance spectroscopy (EIS) measurement between 0.01 and 10⁶ Hz with an AC amplitude of 10 mV and cyclic voltammetry test between 0.005 and 1.5 V at 0.1 mV/s were performed using a PAR Versastat-2 electrochemistry system.

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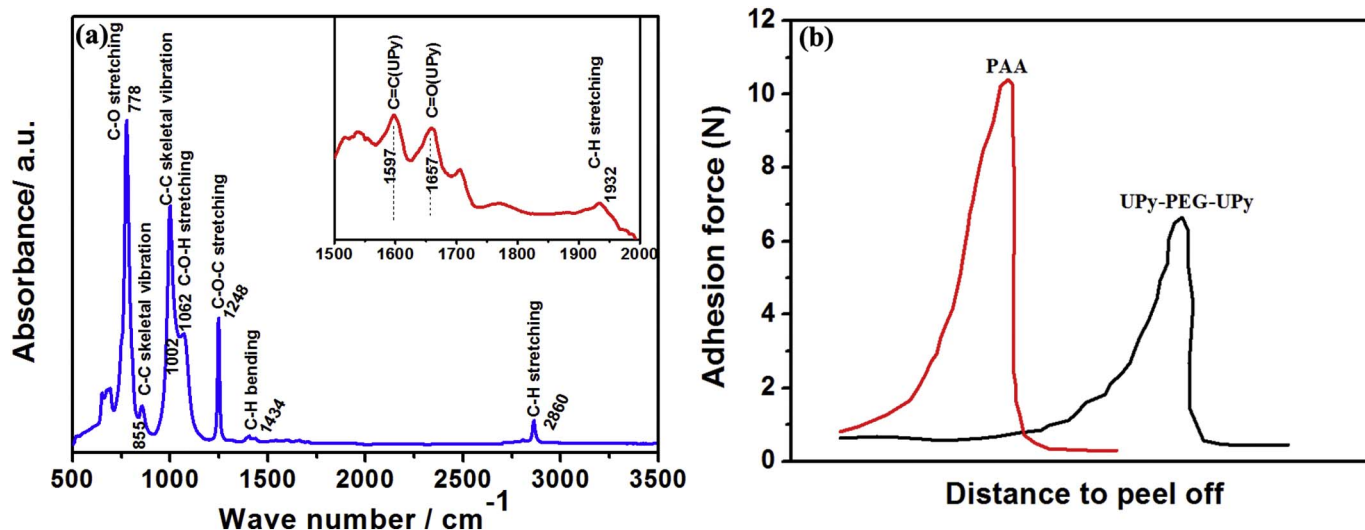


Fig. 1. a) FTIR spectra of as-prepared UPy-PEG-UPy and b) its adhesion force to Si wafer.

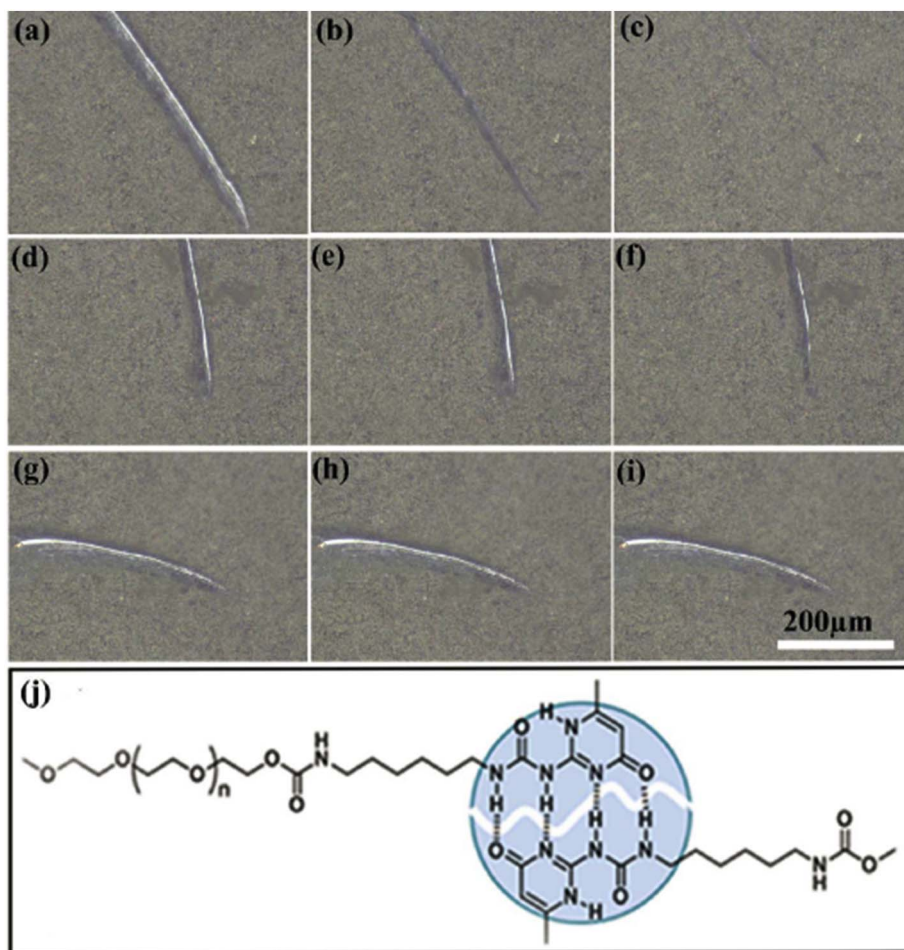


Fig. 2. Optical microscopy image of predefined crack: (a, b, c) as prepared and after 1.5 and 3 h on UPy-PEG-Si-15 electrode, (d, e, f) and (g, h, i) as prepared and after 13 and 25 h on UPy-PEG-Si-15 and PAA-Si-15 electrode, respectively, (j) the proposed mechanism for self-healing of UPy-PEG binders.

3. Results and discussion

Fig. 1 illustrates FTIR spectra of UPy-PEG-UPy. Absorption bands at 778, 855, 1002, 1062, 1248, 1434, and 2860 cm^{-1} correspond to C–O, C–C, C–O–H, C–O–C, and C–H vibration mode of PEG, respectively [22–24]. The disappearance of IR band at 3498 cm^{-1} due to the O–H vibration in PEG [23] suggests the reaction of –OH group with –N=C=O functional group. Two intense bands at 1597 and

1657 cm^{-1} in the insert of Fig. 1 are assigned to C=C and C=O vibration of UPy group [25]. These suggest the successful synthesis of UPy-PEG-UPy. Adhesion force of UPy-PEG-UPy to polycrystalline Si wafer was determined as about 6.5 N less than that of PAA to Si wafer (Fig. 1b) using the same method in [26]. The response of Si electrodes with different binders to a purposely introduced mechanical crack was illustrated in Fig. 2. A mechanical crack was generated on UPy-PEG-Si-15 (Fig. 2a), UPy-PEG-Si-8 (Fig. 2d) and PAA-Si-15 (Fig. 2g) electrodes,

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