

Fall and Rise: Disentangling Cycle Life Trends in Atmospheric Plasma-Synthesized FeOOH/PANI Composite for Conversion Anodes in Lithium-Ion Batteries

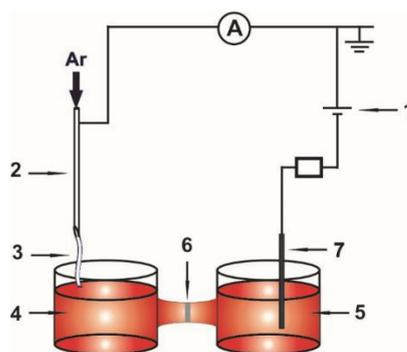
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1 – DC power supply, 2 – a stainless steel capillary tube anode, 3 – plasma discharge, 4 – anolyte, 5 – catholyte, 6 – a glass microfiber filter, 7 – stainless steel mesh cathode

Figure S1. Synthesis setup diagram

XPS measurements were conducted with photoelectron spectrometer Thermo Fisher Scientific Escalab 250Xi with AlK α radiation (photon energy 1486.6 eV). Spectra were recorded in the constant pass energy mode at 50 eV for element core level spectrum and 100 eV for survey, using XPS 650 μ m spot size with total energy of 0.2 eV. To counter the surface charge caused by emitting photoelectrons dual mode charge compensation (a combination of low energy electrons and argon) was used. Investigations were conducted at room temperature in an ultrahigh vacuum of the order of 10⁻⁹ mbar. Peaks were fitted with a product of asymmetric Gaussian and Lorentzian lineshape.

XRD powder X-ray diffraction (Bruker D2 Phaser with the following conditions: CoK α 1+2 radiation with 30 kV/10 mA, $\lambda_{\text{CoK}\alpha 1} = 1.78897 \text{ \AA}$ and $\lambda_{\text{CoK}\alpha 2} = 1.79285 \text{ \AA}$, the position sensitive detector, the Bragg-Brentano parafocusing geometry, rotation speed = 20 rpm, range of diffraction angles $2\theta = (5-75)^\circ$ with a step size of 0.02 $^\circ$, point exposure = 0.5 s, air, $T = 25 \text{ }^\circ\text{C}$).

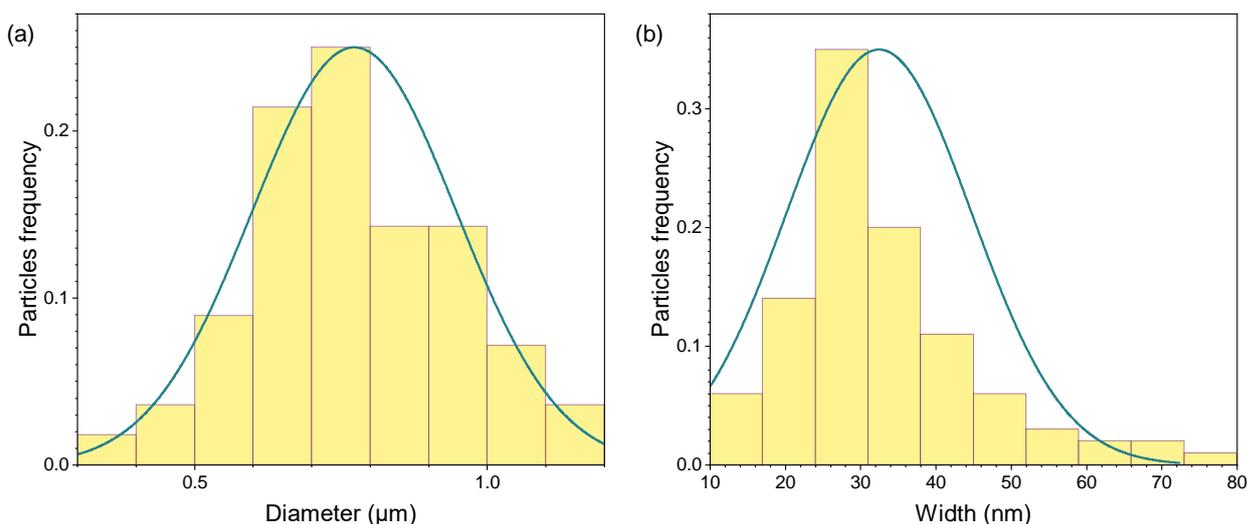


Figure S2. FeOOH/PANI powder particles sizes distribution estimated from SEM images: diameter of urchin-like spheres (a) and width/thickness of needles (b).

The XRD pattern of the synthesized material is shown in Figure S3. The diffractogram does not contain any peaks related to PANI due to the high amorphous nature of the material. Nevertheless, the diffraction peaks correspond to those of schwertmannite (PDF 47-1775), including the peaks at 20.17° , 30.49° , 33.54° , 41.18° and 52.44° . The shift of the peaks with respect to the reference is caused by the different material of the X-ray tube anode and the different X-ray lengths (1.5406 \AA for copper vs 1.7902 \AA for cobalt).

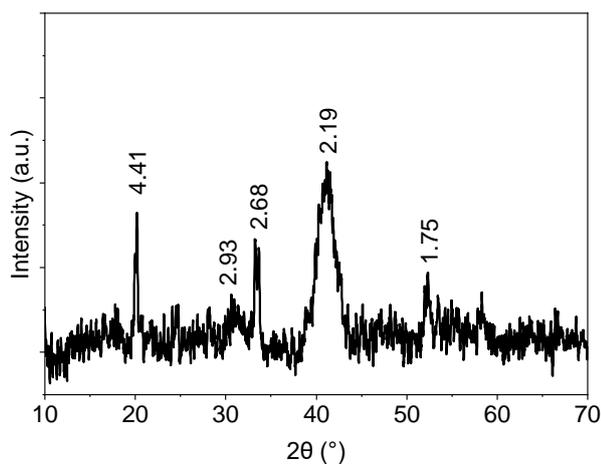


Figure S3. XRD of FeOOH/PANI particles labeled with d-spacing (\AA) values.

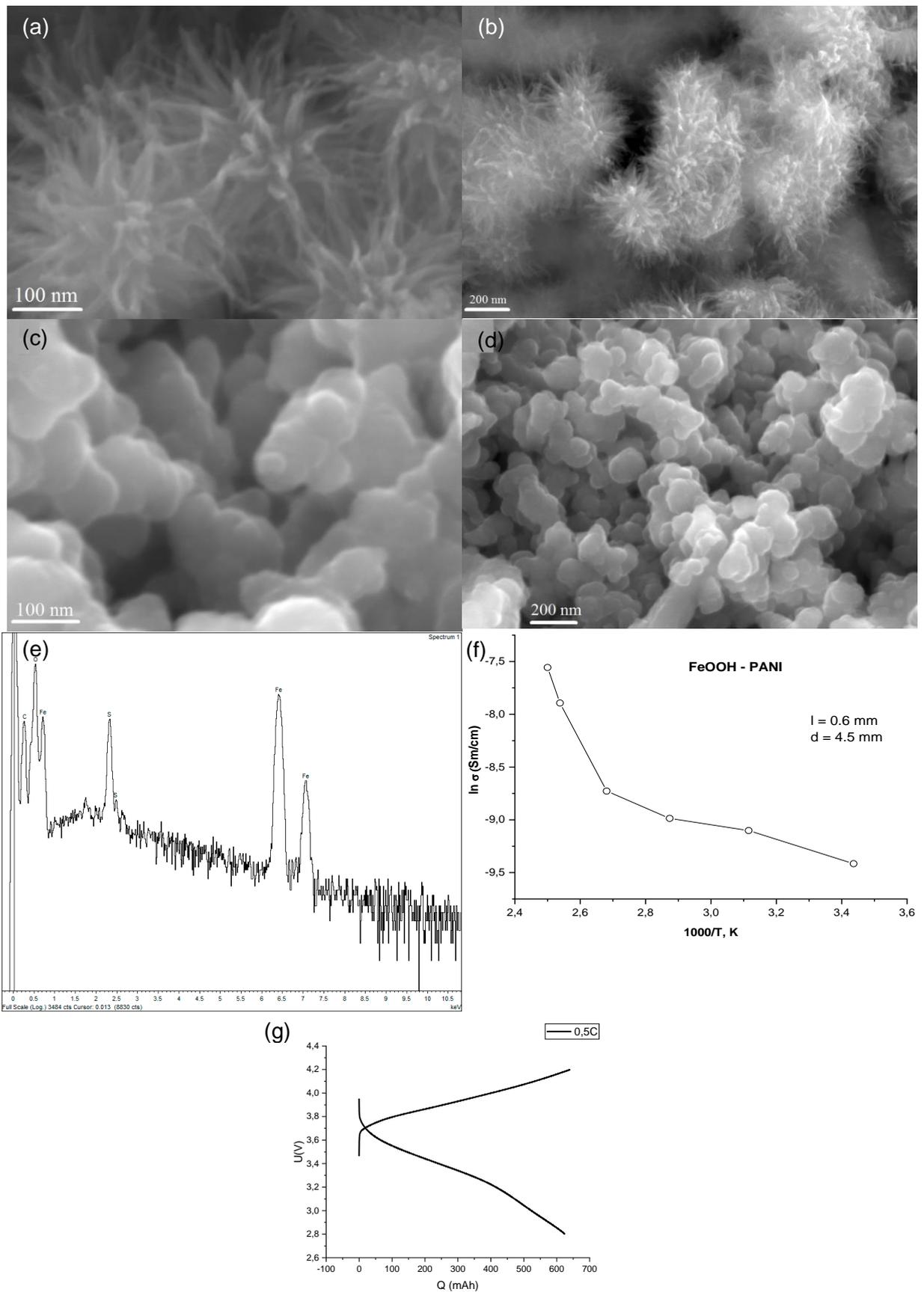


Figure S4. SEM images of plasma solution synthesized FeOOH (a, b) and PANI (c,d) nanoparticles; EDX spectra of FeOOH/PANI composite (e); electrical conductivity temperature dependence of FeOOH/PANI composite (f); charge-discharge curve of the NMC532 - Graphite full cell at a C/2 rate (g).

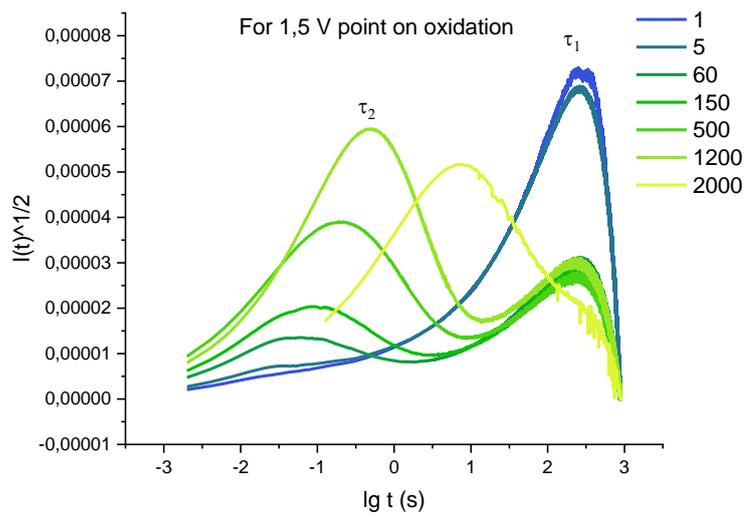


Figure S5. Cottrell function plot for the current transient versus the decimal logarithm of time

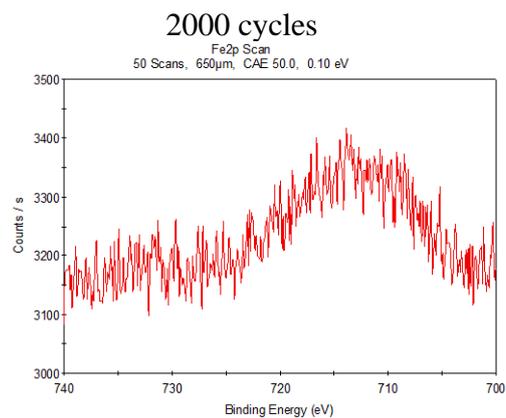
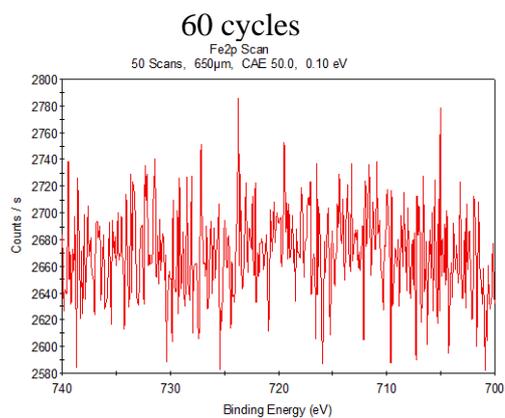
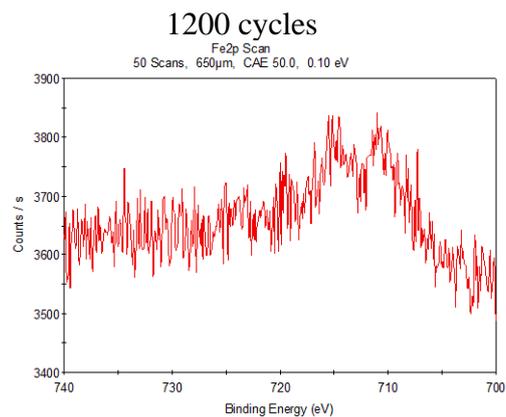
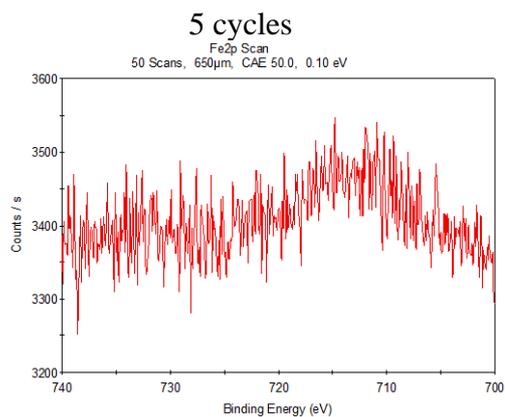
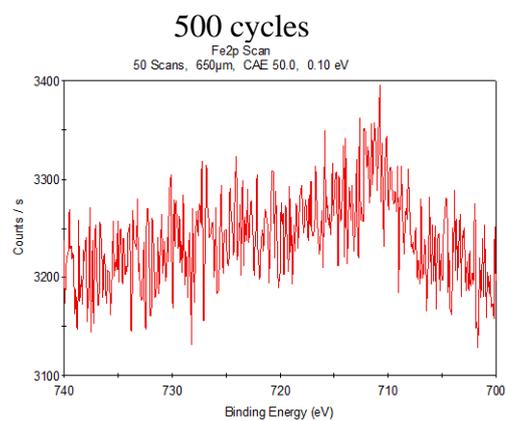
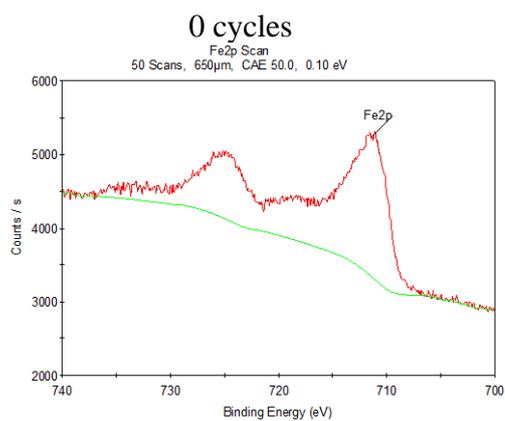


Figure S6. XPS spectra of Fe 2p

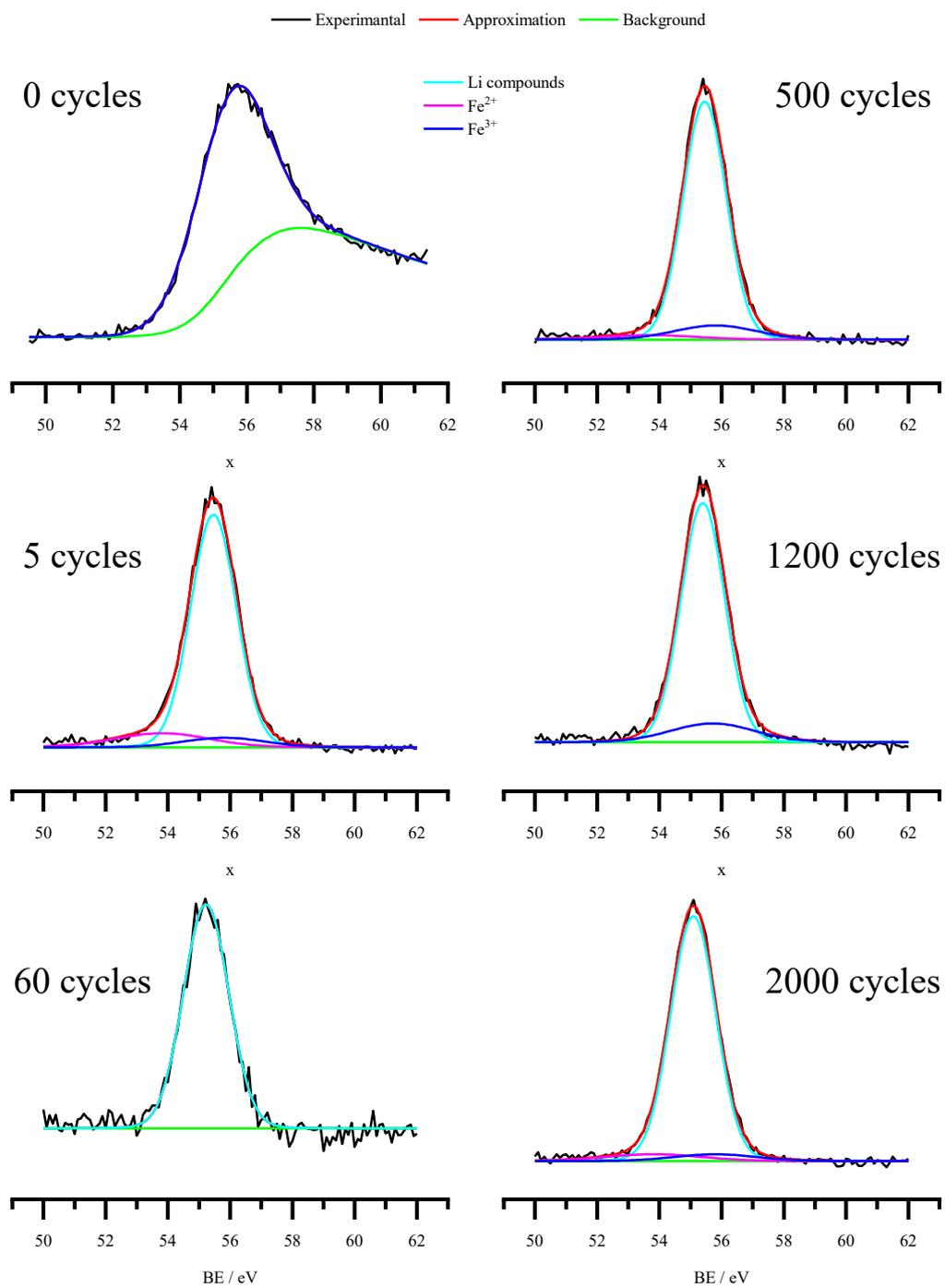


Figure S7. XPS spectra of Li 1s + Fe 3p

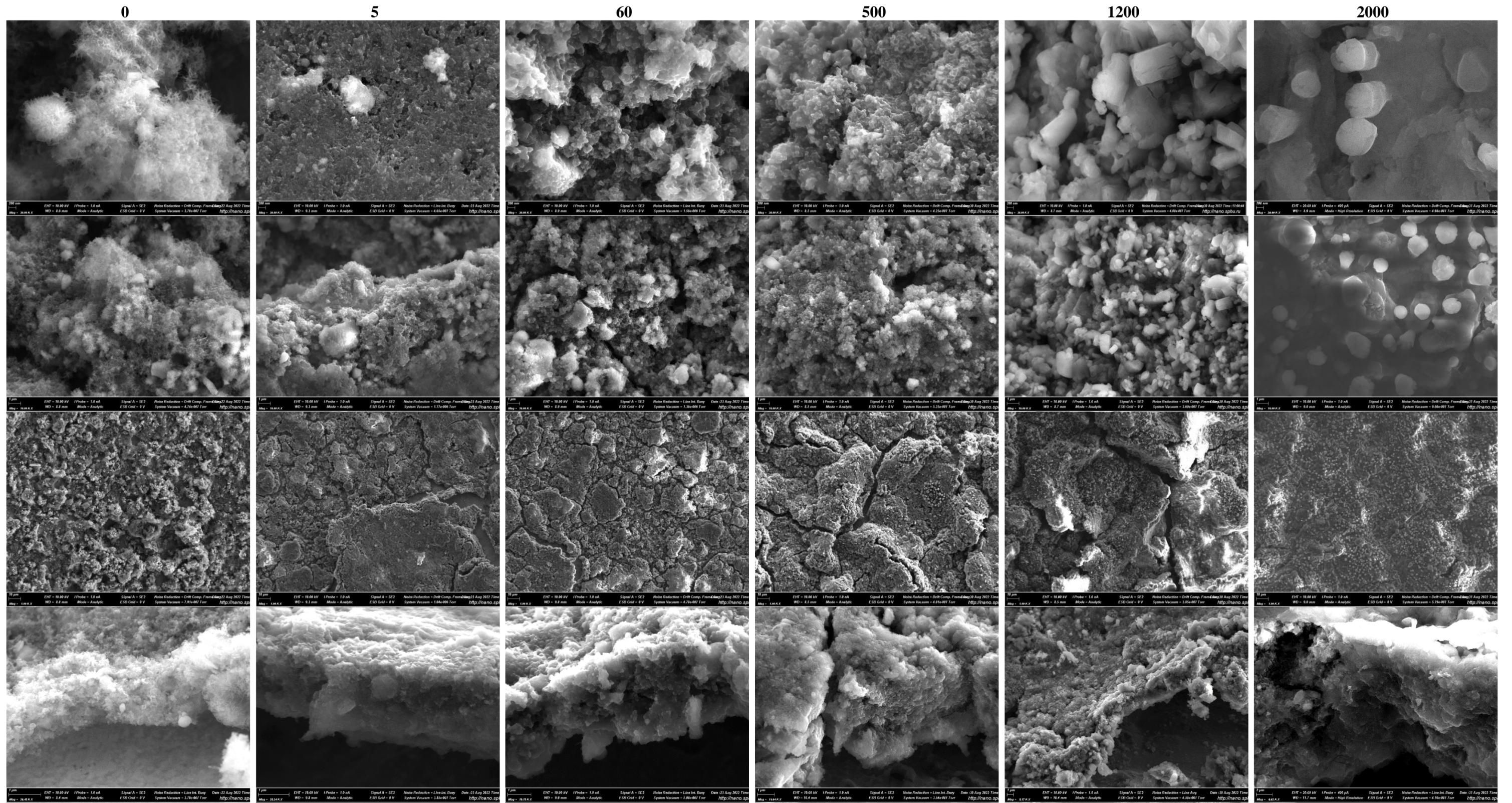


Figure S8. Evolution of the electrode surface during 2000 cycles