

Supporting Information

Pyrite FeS₂-C Composite as a High Capacity Cathode Material of Rechargeable Lithium and Lithium-Ion Batteries

Dat T. Tran,¹ Hong Dong,² Scott D. Walck,² and Sheng S. Zhang^{*,1}

¹Sensors and Electron Devices Directorate, U.S. Army Research Laboratory, Adelphi, MD 20783-1138, USA. Email: shengshui.zhang.civ@mail.mil; shengshui@gmail.com

²Weapons and Materials Research Directorate, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005-5069, USA

Structural characterizations of FeS₂-C composites

Elemental analysis service was provided by Micro-Analysis, Inc. (Wilmington, DE). Powder X-ray diffraction (XRD) was performed on an X-ray diffractometer (Rigaku Ultima III) with Cu-K α radiation ($\lambda = 1.5418 \text{ \AA}$) from 20° to 55° at a scanning rate of 1° min⁻¹. Raman spectrum was acquired by a Renishaw inVia Raman microscope and the data were analyzed using a WiRE 4.1 software. Specific surface area was determined by the Brunauer–Emmett–Teller (BET) method using a Micromeritics physisorption analyzer (TriStar II 3020 v1.03). Morphology was observed and analyzed using a Quanta 200F scanning electron microscope (SEM) and a JEOL 2100F transmission electron microscope (TEM), respectively. In order to perform scanning transmission electron microscopy (STEM) observation, the sample particles were dispersed in ethanol and then drop-casted on the TEM grids with holey carbon support films. In order to observe the cross-sectional view of the particles, the particles were embedded in EPO-FIX embedding epoxy resin (Electron Microscopy Sciences) and cured at 60 °C for three hours. The embedded resin was cross-sectioned using a Leica microtome. The sliced thin sections with thickness ~100 nm were collected on the TEM grids with holey carbon support films. The particles and cross sections of particles were investigated using a JEOL 2100F scope in the STEM mode operating at 200 kV. Bright Field (BF) STEM image was acquired using a JEOL BF detector, and High Angle Annular Dark Field (HAADF) image was acquired with a Gatan 806 HAADF detector operating with a collection angle range of 48 to 168 mrad. The Energy-Dispersive X-Ray Spectroscopy (EDS) spectra of the particles and the cross sections were collected on an HAADF image using the Gatan system. The compositional maps based on spectra imaging were constructed using AXSIA software.

Table S1. Composition and specific surface area of FeS₂ and FeS₂-C composites

Sample code	C, wt.% by elemental analysis	Specific surface area, m ² g ⁻¹
FeS ₂	1.93	3.86
FeS ₂ -C-I	13.36	10.17
FeS ₂ -C-II	18.68	27.06

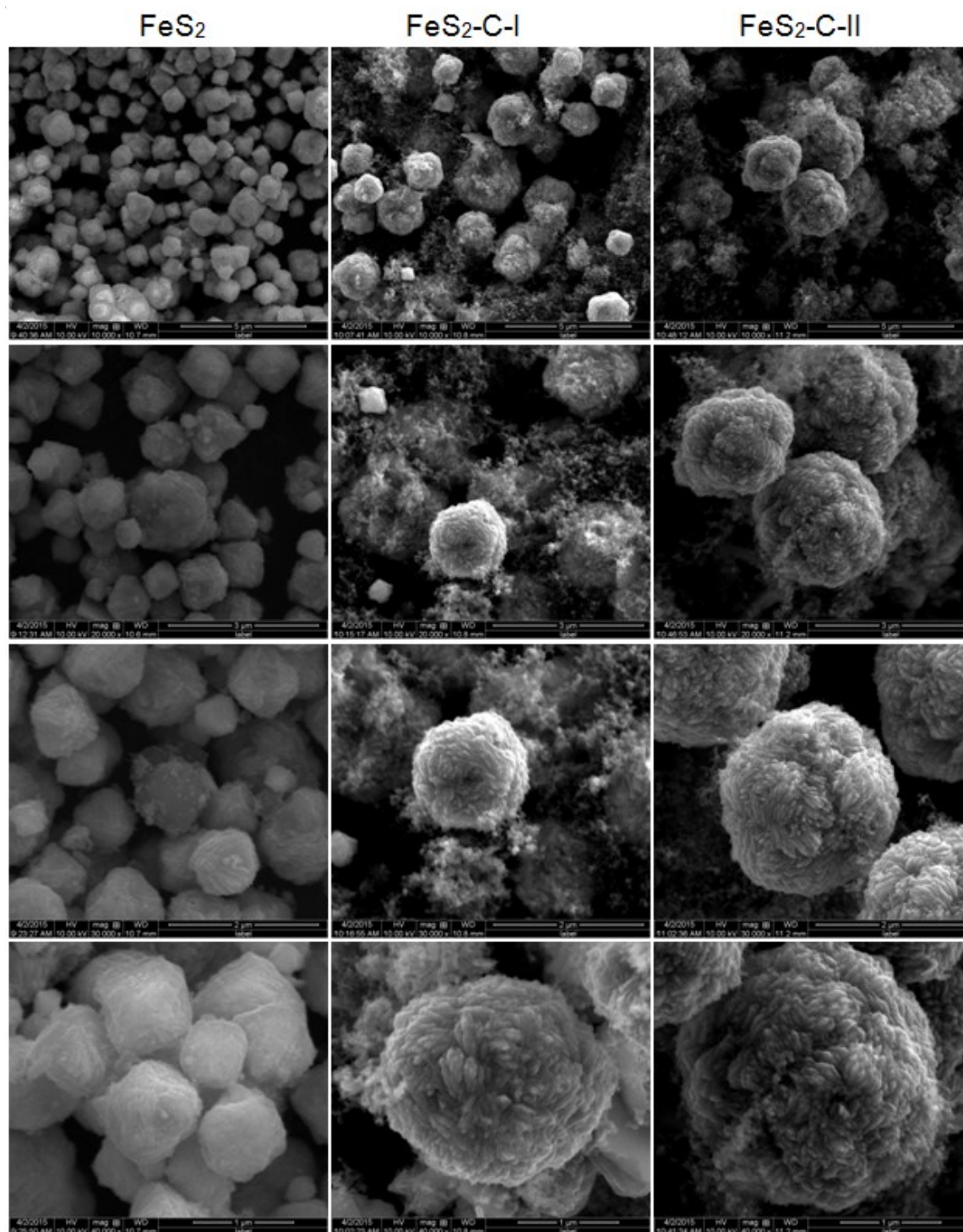


Figure S1. SEM images at different magnifications of FeS₂, FeS₂-C-I, and FeS₂-C-II.

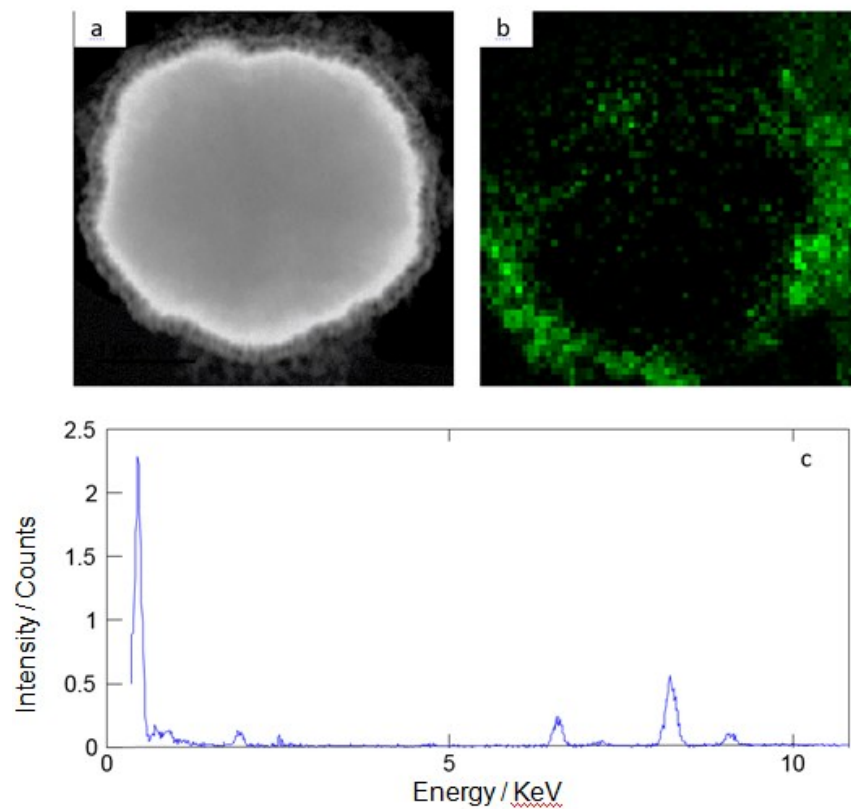


Figure S2. (a) STEM HAADF image of a $\text{FeS}_2\text{-C-II}$ particle, (b) a typical composition map where the green area represents carbon as the main component, and (c) EDS spectrum of the green area in b.

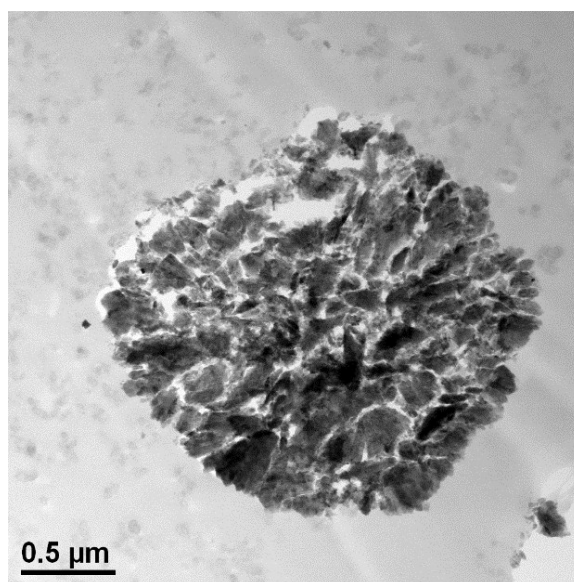


Figure S3. STEM BF image of the cross-section of a $\text{FeS}_2\text{-C-II}$ particle.