INESS mesc-is 2023

One-pot synthesis of free-standing LiCoPO₄/C composite nanofibers as highvoltage cathode materials for lithium-ion batteries

Ayaulym Belgibayeva^{1,2,*}, Samal Berikbaikyzy, Zhumabay Bakenov^{1,2}, and Izumi Taniguchi³

¹National Laboratory Astana, Nazarbayev University, 53 Kabanbay Batyr Ave., Astana, Kazakhstan

²Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, 53 Kabanbay Batyr Ave., Astana, Kazakhstan

³Department of Chemical Science and Engineering, Tokyo Institute of Technology, Tokyo 152-8552, Japan

Introduction

Lithium cobalt phosphate (LCP) is a high-voltage lithium-ion cathode material which appears to be appealing due to its high theoretical capacity of 170 mAh g^{-1} with higher energy density compared to lithium iron phosphate, as its redox potential is 4.8 V (vs. Li/Li⁺) [1]. The main challenge limiting the practical capacity and cyclability of LCP is its low electrical conductivity.

In this work, we propose one-pot synthesis of LCP nanoparticles incorparated within carbon fiber matrix by electrospinning with heat treatment to improve the electrical conductivity of the cathode material. Pre-oxidation temperature of the precursor fibers was varied to find the optimal carbon content for the best electrochemical performance.

Experimental details

Electrospinning solution was prepared as reported elsewhere [2] with the addition of stoichiometric amount of lithium nitrate and electrospun under voltage of 18 kV, tip-to-collector distance of 10 cm, flow rate of 1 mL h⁻¹, making use of a drum-type collector. Fibers were dried at 150 °C, pre-oxidized at different temperatures, and heat-treated at 700 °C in N₂ atmosphere. The crystal structure and the morphology of nanofibers were studied by X-Ray diffraction (XRD, Miniflex, Rigaku) and scanning electron microscopy (SEM, Crossbeam500, Zeiss), respectively. The carbon content was determined by CHNS analysis.

Results and Discussion

Figure 1a shows XRD patterns of samples annealed in N_2 at 700 °C after pre-oxidation at different temperatures. Formation of orthorhombic LiCoPO₄ with Pnma(62) space group can be observed in all three samples with a small impurity peak at about 22°, which decreases with increasing the pre-oxidation temperature.

Figure 1b shows the SEM images of prepared samples. In this case, several differences have been observed, including particle formation. Fibers of sample prepared by pre-oxidation at 300 °C are more decorated with nanoparticles, while surface of samples prepared by pre-oxidation at 330 °C and 350 °C is more smooth and uniform, suggesting encapsulation of LCP nanoparticles within the fiber matrix.



Figure 1. (a) XRD patterns and (b) SEM images of samples pre-oxidized at different temperatures.

The elemental composition of three samples determined by CHNS analysis is shown in **Table 1**. The difference in the pre-oxidation temperatures resulted in the differences in the carbon contents and C/N ratio of samples.

Table 1	Flemental	composition	determined	by CHNS
I abic I	Licincintai	composition	ucicilinicu	Uy CIIINS.

Sample	C, wt.%	N, wt.%	C/N ratio
300 °C	17.0	2.8	6.0
330 °C	16.7	2.9	5.7
350 °C	11.5	2.3	5.1

Electrochemical properties of the obtained materials will be presented at the conference.

Acknowledgements

This research was funded by the project AP13068219 "Development of multifunctional free-standing carbon composite nanofiber mats" from the Ministry of Education and Science of the Republic of Kazakhstan.

References

[1] K. Amine, H. Asuda and M. Yamachi, J. Electrochem. Soc., 2002.

[2] A. Belgibayeva, M. Rakhatkyzy, A. Adi, I. Taniguchi, ChemElectroChem. 9 (2022) e202200458.



Dr. Ayaulym Belgibayeva received her Ph.D. in Chemical Science and Engineering from Tokyo Institute of Technology, Tokyo, Japan, under the supervision of Prof. Izumi Taniguchi in 2021. She has joined Battery Research Group of Prof. Bakenov at Nazarbayev University, Kazakhstan, as a Postdoctoral Researcher and started new project on the development of multifunctional nanofibers as a PI. Her current research interests include development of nanocomposites for energy storage applications.

Presentating author: Ayaulym Belgibayeva, e-mail: ayaulym.belgibayeva@nu.edu.kz tel: +7776668328