ELECTROCHEMICAL PROPERTIES OF $Ba_2HoCu_3O_7$

MARIIA-SUZANNA TEPLINSKA, OKSANA ZAREMBA, PAVLO DEMCHENKO, VASYL KORDAN, ROMAN GLADYSHEVSKII

Ivan Franko National University of Lviv, Ukraine

The ceramic phase $Ba_2HoCu_3O_7$ was tested as potential cathode material of a lithium-ion battery. A single-phase polycrystalline sample was synthesized via solid-state reaction and characterized by XRD, SEM, and EDX. Electrochemical lithiation in a $Ba_2HoCu_3O_7$ cell preserved the initial structure with a volume expansion of $\Delta V/V = 0.21\%$. Up to 0.63 Li per formula unit was intercalated, and the battery showed cycling stability over 50 cycles.

Keywords: complex cuprates, solid-state synthesis, $Ba_2HoCu_3O_7$, YBCO structure, electrochemical lithiation

The AO–R_2O_3–CuO systems, where *A* is an alkaline-earth and *R* a rare-earth metal, started to be intensively investigated after the discovery of the phenomenon of high-temperature superconductivity in layered cuprates. One of the first and assuredly the most studied compound was the $Ba_2YCu_3O_7$ (YBCO) phase, whose orthorhombic polymorphic modification is characterized by a transition temperature to the superconducting state close to 100 K at ambient pressure. According to Pearson's Crystal Data [1], the existence of YBCO phases has been reported in all BaO–R_2O_3–CuO systems, excluding those with radioactive Pm. Among the promising fields of application are superconducting magnets, zero-resistance cables, quantum computers, various sensors, etc. Another up and coming area for the implementation of YBCO-type cuprates may be energy-saving technologies, considering the peculiarities of their crystal structure, namely the presence of voids and channels where lithium atoms can be intercalated/deintercalated during electrochemical processes. The aim of the present work was the synthesis of pure $Ba_2HoCu_3O_7$ cuprates and investigation of its electrochemical properties.

A polycrystalline sample with the nominal composition $Ba_2HoCu_3O_7$ was synthesized using the solid-state reaction method. High-purity powders of barium carbonate, holmium and copper oxides served as starting materials. The initial powders were manually mixed and ground for 10 minutes to ensure homogeneity. The resulting mixture was then subjected to thermal treatment in a corundum crucible in a muffle furnace at 900°C for 24 hours in an air atmosphere, facilitating the decomposition of the carbonate. The obtained mixture was re-ground, pressed into a pellet, and sintered under identical conditions. To control the composition and surface morphology of the samples before and after lithiation, scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) were used (Tescan Vega 3 LMU, Oxford Instruments energy-dispersive X-ray analyser, Aztec ONE system). X-ray diffraction (XRD) data were collected on a STOE Stadi P diffractometer (Cu $K\alpha_1$ radiation). FullProf software using the Rietveld method was applied for the crystal structure analysis. Electrochemical lithiation was carried out in the galvanostatic mode (2-electrode Swagelok-type cell).

The ceramic single-phase $Ba_2HoCu_3O_7$ sample was tested as cathode material of a lithium-ion battery, where commercial metallic lithium was used as anode. The processes of intercalation/deintercalation of lithium atoms proceed without changing the crystal structure (Table 1). The increase of the cell volume $\Delta V/V$ (0.21%) indicates the formation of a solid solution of inclusion type during the lithiation. As a result of the electrochemical reaction, the $Ba_2HoCu_3O_7$: Li phase was obtained. The maximum amount of intercalated Li was 0.63 per formula unit (f.u.). 50 discharge/charge cycles were performed.

Table 1. Experimental characteristics of the $Ba_2HoCu_3O_7$ phase (structure type $Ba_2YCu_3O_7$, Pearson symbol *oP*13, space group *Pmmm*) before and after lithiation.

$Ba_2HoCu_3O_7$			$Ba_2HoCu_3O_7$:Li		
XRD	EDX		XRD	EDX	
	Element	Content (at. %)		Element	Content (at. %)
a = 3.8208(2) Å b = 3.8821(2) Å c = 11.6791(8) Å V = 173.237(18) Å^3 R_I = 0.117, R_p = 0.0397, R_{wp} = 0.0547, R_{exp} = 0.0533, χ^2 = 1.05	Ba Ho Cu O	16.9 7.4 25.1 50.6	a = 3.82455(15) Å b = 3.88352(17) Å c = 11.6879(5) Å V = 173.598(13) Å^3 R_I = 0.0473, R_p = 0.0323, R_{wp} = 0.0433, R_{exp} = 0.0375, χ^2 = 1.33	Ba Ho Cu O	17.6 9.0 23.1 50.3

1. *Villars, P., Cenzual, K. (Eds.), Pearson's Crystal Data, Crystal Structure Database for Inorganic Compounds // ASM International, Materials Park (OH). – 2023/2024.* *https://www.asminternational.org/materials-resources/online-databases/pearsons-crystal-data-crystal-structure-database-for-inorganic-compounds/?srsltid=AfmBOoonfzVrKnDGWDtyiqhDUfgS0zdyjJHqoeWnzPq02AVUinJ90TV4*