Секция 7. Химия и химическая технология на иностранном языке (английский)

Characteristic	01	02	03	O4	05	O6	07	08
СР	-14	-28	-28	-13	-30	-16	-19	-18
РР	-42	-50	-50	-26	-43	-37	-31	-36
						•		

 Table 1.
 Low-temperature properties of motor oils

Table 2. Physicochemical characteristics

Table 2. Thysicochemical characteristics											
Characteristic	01	O2	O3	O4	05	O6	O7	08			
Mass fraction of sulfur, mg/kg	1993	1966	2030	5851	2156	2104	6723	2930			
Density at 20 °C, kg/m ³	838,3	837,9	838,9	878,6	846,1	864,4	879,2	854,3			
Kinematic viscosity at 20 °C, mm ² /s	118,8	184,8	174,6	234,8	273,1	281,8	396,4	235,9			
Dynamic viscosi- ty at 20 °C, Pa/s	99,6	154,9	146,5	206,3	231,0	243,6	348,5	201,6			

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CRYSTALLOGRAPHIC INSIGHTS INTO HYDROTHERMALLY SYNTHESIZED TETRAGONAL BARIUM TITANATE NANOPARTICLES

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The escalating demand for high-performance piezoelectric perovskite materials, integrated into several technologies as sensors, actuators, ultrasonic devices, and thermal imaging, promotes researchers worldwide to optimize efficiency and explore eco-friendly alternatives to lead-based perovskites, addressing this growing demand for piezoelectrics. Therefore, barium titanate (BT, Ba-TiO₂) has emerged as a promising solution due to its dielectric properties and biocompatibility [1]. Herein, our work employs X-ray diffraction (XRD) on hydrothermally synthesized BT nanoparticles to investigate its crystal structure and piezoelectric properties. The focus is on understanding how geometric features influence the BT performance after hydrothermal synthesis under elevated temperature and pressure, contributing new insights to the existing body of knowledge in this field.

BT nanoparticles were synthesized through a hydrothermal process using barium hydroxide octahydrate and titanium dioxide, then XRD analysis to identify phase composition and crystal structure.

Fig. 1 shows that the XRD pattern was agreed well with the reference card (COD, No. 1507756, BaTiO₃), indicating a pure phase without impurities. The observed peak shoulder around $2\theta = 45^{\circ}$ confirmed the tetragonal crystal structure. Analysis of lattice parameters (a = 3.9979, b = 3.9979, c = 4.0228 A) was done. Furthermore, crystallite size = 67.356 nm, and lattice strain = 0.00215 were determined.

In Fig. 2, the simulation model of refining crystallographic data results revealed a contrast in geometric symmetry between normal and distorted tetragonal barium titanate. It might be the impact of emergent oxygen vacancies in the crystal lattice during hydrothermal synthesis under elevated temperature and pressure, which led to the formation of Ba²⁺ vacancies for maintaining the lattice electroneutrality, resulting in lattice deformation, octahedron tilting, and Ba²⁺ displacement.

This phenomenon enlarges charge separation, increasing polarizability – an essential factor for

piezoelectric applications. Moreover, we assume the accumulation of oxygen ions on one-face of the crystal lattice, altering its chemistry and may have a potential effect on catalytic and piezoelectric properties, which requires further study.



Fig. 1. XRD patterns of hydrothermally synthesized barium titanate



Fig. 2. Comparison between the simulated model of crystal structure of tetragonal BaTiO₃ hydrothermally synthesized and the reference one from different viewing sides

References

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TAILORED TETRAGONAL BARIUM TITANATE NANOPARTICLES FROM BARIUM CARBONATE PRECURSOR VIA HYDROTHERMAL METHOD

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Barium titanate (BaTiO₃) stands as a fascinating ferroelectric material due to its remarkable dielectric, piezoelectric, and pyroelectric properties, reflecting its high compatibility for diverse applications such as capacitors, sensors, and actuators. However, the synthesis of BaTiO₃ nanoparticles with the requisite attributes, including high purity, uniform size, and controlled crystal structure, persists as a ubiquitous challenge [1]. Among the various methodologies for producing BaTiO₃ n anoparticles, the hydrothermal method has gained prominence owing to its simplicity, scalability, and environmental friendliness [2]. Therefore, our research aims to synthesize tetragonal BaTiO₃ from BaCO₃ under elevated temperature and pressure via a hydrothermal reactor with the merit of a more uniform particle size distribution and less energy consumed than the solid-state approach [3].

BaTiO₃ nanoparticles were synthesized through a reaction of 3.25 g barium carbonate and 0.685 g titanium dioxide in a water-ethanol solution with sodium hydroxide. Following a 24 h hydrothermal



Fig. 1. XRD patterns of hydrothermally synthesized barium titanate nanoparticles