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GB/T 46514-2025

**Test method for cathode materials of lithium ion battery -
Determination of crystal structure - X-ray diffraction method**

锂离子电池正极材料检测方法 晶体结构的测定 X射线衍射法

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Foreword

This document complies with the provisions of GB/T 1.1-2020 "Standardization Work Guidelines Part

1. Structure and Drafting Rules of Standardization Documents". Drafting. Please note that some content in this document may involve patents. The issuing organization of this document assumes no responsibility for identifying patents. This document was proposed by the China Nonferrous Metals Industry Association. This document is under the jurisdiction of the National Technical Committee on Standardization of Nonferrous Metals (SAC/TC243). This document was drafted by: Guangdong Bangpu Recycling Technology Co., Ltd., Beijing Dangsheng Materials Technology Co., Ltd., and Shenzhen Defang Nano Technology Co., Ltd., Guizhou Zhenhua New Materials Co., Ltd., GEM (Wuxi) Energy Materials Co., Ltd., Sichuan Provincial Product Quality Supervision and Inspection Institute, National Standard (Beijing) Inspection and Certification Co., Ltd., Hubei Wanrun New Energy Technology Co., Ltd., Yichang Bangpu Recycling Technology Co., Ltd. Technology Co., Ltd., Jinchuan Group Co., Ltd., Zhejiang Huayou Cobalt Co., Ltd., Hefei Guoxuan High-Tech Power Energy Co., Ltd. BASF Shanshan Battery Materials Co., Ltd., Hunan Changyuan Lithium Technology New Energy Co., Ltd., and Guolian Automotive Power Battery Research Institute Co., Ltd. Company, Yichun Lithium Battery Industry Research Institute (Jiangxi Provincial Lithium Battery Product Quality Supervision and Inspection Center), Jiangxi Ganfeng Lithium Group Co., Ltd., Yichun Springtime Gifts High-Tech Materials Co., Ltd. The main drafters of this document are. Yu Haijun, Xie Yinghao, Cui Fan, Liu Zhipeng, Fu Haikuan, Wang Yujiao, Jin Qingqing, Tan Meijuan, Luo Lin, and Xu Kaihua. Zhang Xicui, Wang Mengyuan, Gui Fanghai, Deng Bei, Wu Xiaoping, Chen Sibe, Dai Zehua, Deng Zhibin, Xu Jiale, Ma Yanhui, Luo Jing, Liu Chenfei, Yang Cheng Wan Yumei, Li Xiaobing, Li Qiang, Zhang Liping, Yuan Huan. Testing methods for positive electrode materials of lithium-ion batteries Determination of crystal structure by X-ray diffraction

1 Scope

GB/T 46514-2025 is the Chinese national standard covering the crystal structure of a

cathode powder by XRD - the specimen preparation and the preferred orientation it must avoid, the scan conditions, the lattice parameters and the cation mixing between lithium and nickel sites that governs how the material performs. First edition, under the China Nonferrous Metals Industry Association. In force from 1 May 2026. Issued on 5 October 2025, it has been in force since 1 May 2026.

This document describes a method for determining the crystal structure of lithium-ion battery cathode materials using X-ray diffraction. This document applies to the crystal structure of lithium-ion battery cathode materials such as lithium nickel cobalt manganese oxide, lithium iron phosphate, lithium cobalt oxide, lithium manganese oxide, and lithium manganese iron phosphate. The determination.

2 Normative references

The contents of the following documents, through normative references within the text, constitute essential provisions of this document. Dated citations are not included. For references to documents, only the version corresponding to that date applies to this document; for undated references, the latest version (including all amendments) applies. This document.

GB/T 8170 Rules for rounding off numerical values and the representation and determination of limiting values

GB/T 30904 X-ray diffraction method for crystal structure analysis of inorganic chemical products JJG629 Verification Procedure for Polycrystalline X-ray Diffractometer JY/T 0587 General Rules for Polycrystalline X-ray Diffraction Methods

3 Terms and Definitions

The terms and definitions defined in GB/T 30904 and JY/T 0587, as well as the following terms and definitions, apply to this document.

3.1 step size The angular interval between two adjacent data points in a diffraction pattern.

3.2 Weighted pattern residual variance factor R-weighted pattern RWP A parameter that measures the degree of agreement between calculated XRD patterns and measured XRD patterns.

3.3 Difference curve The curve plotted as the difference between the calculated XRD pattern and the measured XRD pattern varies with the diffraction angle.

4 Principles

4.1 X-ray diffraction method When X-rays pass through a crystal, diffraction occurs, and the diffraction pattern is related to the ordered structure of the crystal, reflecting the regularity of the crystal structure. The interplanar spacing and X-ray wavelength conform to the Bragg

formula, see formula (1). $2\delta h k l \sin \theta_{hkl} = n\lambda$ (1)

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