Full Paper

Reference Object Identifier - ROI: jbc-02/17-51-7-86 Publication is available for discussion in the framework of the on-line Internet conference "Butlerov readings". http://butlerov.com/readings/ Submitted on Jule 26, 2017.

The method of calculation of crystallographic characteristics of graphite

© Anna N. Popova

Federal Research Center on Coal and Coal Chemistry, Siberian Branch, Russian Academy of Sciences. Sovetskiy pr, 18. Kemerovo, 650000. Russia. E-mail: h991@yandex.ru

Keywords: XRD analysis, crystal structure, graphite.

Abstract

The X-ray diffraction method is one of the most common, and even non-destructive, methods that characterize carbon materials and composites based on them. X-ray diffraction is used to study the phase composition of the samples, to carry out the qualitative and quantitative composition of certain phases, to estimate the crystallographic structural characteristics of the carbon materials. The article is devoted to the results of calculation of the main structural parameters of graphites that have undergone various treatments. The main characteristics of the crystal structure of the samples are the interplanar spacing (d00l), the dimensions of the structural components (La and Lc), and the degree of ordering. To describe the heterogeneity of the samples phase composition, the obtained data are compared with the main crystallographic reflections of the (001) series, which corresponds to the main plane of graphite. It is shown that the reflections (002), (004) and (006) are superposition of the components characterizing the individual structural phases of the investigated samples. The decomposition of the reflexes into structural components makes it possible to introduce an additional characteristic of the sample-the phase relationship, which makes it possible to better characterize the crystal structure of the samples in the case when their structural characteristics are close.

References

- [1] V.A. Liopo, V.V. Voyna. X-ray diffractometry: Proc. allowance. Grodno: Publishing house of the State University of Grodno. 2003. 171p. (russian)
- [2] G.P. Khokhlova, Ch.N. Barnakov, V.Yu. Malysheva, et al. Effect of heat treatment conditions on the catalytic graphitization of coal-tar pitch. Solid Fuel Chemistry. 2015. Vol.49. No.2. P.66-72.
- [3] G.P. Khokhlova, Ch.N. Barnakov, A.N. Popova, et al. Influence of carbon additives on the thermal transformation of coal pitch. Coke and Chemistry. 2015. Vol.58. No.7. P.268-274.
- [4] G.P. Khokhlova, C.N. Barnakov, and A.N. Popova. Carbonization of coal pitch with graphite additives. Coke and Chemistry. 2016. Vol.59. No.1. P.27-34.
- [5] Ch.N. Barnakov, G.P. Khokhlova, A.N. Popova, S.A. Sozinov, Z.R. Ismagilov. XRD characterization of the structure of graphites and carbon materials obtained by the low-temperature graphitization of coal tar pitch. Eurasian Chemico-Technological Journal. 2015. Vol.17. No.2. P.87-93.
- [6] G.P. Khokhlova, V.Yu. Malysheva, Ch.N. Barnakov, et al. Influence of the nature and amount of the catalyst on the phase structure of the carbon material obtained by low-temperature catalytic graphitization of coal tar pitch. Bulletin of the Kuzbass State Technical University. 2013. No.5. P.21-24. (russian)
- [7] S.V. Stakhanova, M.V. Astakhov, A.A. Klimont, I.S. Krechetov, A.T. Kalashnik, R.R. Galymzyanov and K.A. Semushin. Polyaniline composites based on porous fibrous carbon materials for supercapacitor electrode structures. Butlerov Communications. 2015. Vol.41. No.1. P.130-137. ROI: jbc-02/15-41-1-130
- [8] E.S. Vavilov, and I.N. Kovalev. Effect of synthesis condition on the morphology of obtained carbon materials. Butlerov Communications. 2015. Vol.44. No.12. P.196-198. ROI: jbc-02/15-44-12-196
- [9] Brief chemical encyclopedia. Moscow: Soviet Encyclopedia. 1967. Vol.5. P.303-313. (russian)
- [10] A.S. Fialkov. Carbon graphite materials. *Moscow: Publishing house "Energia"*. 1979. 319p. (russian)
- [11] O.P. Yatsyuk. Influence of conditions of thermochemical treatment of natural graphite on its crystal structure and electrophysical properties. Solid Fuel Chemistry. 1990. No.6. P.104-108. (russian)
- Yu.A. Dvadin. Graphite and its inclusion compounds. Soros Educational Journal. 2000. Vol.6. No.10. [12] P.43-49. (russian)
- [13] ICDD, PDF-2. 2011 (Database), edited by Dr. Surya Kalakkodu, International Centre for Diffraction Data. Newtown Square, PA, USA.