

The study of the structural characteristics of carbon Materials by mean of XRD analysis

© Anna N. Popova,*⁺ Chingiz N. Barnakov, Galina P. Khohlova

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

*Supervising author; ⁺Corresponding author

Keywords: coal pitch, graphite additives, graphitization, X-ray diffraction analysis.

Abstract

The powder X-ray diffraction method is one of the important methods for describing the structural characteristics of carbon materials, the main advantage of which is that this method is non-destructive. It is used to perform qualitative and quantitative X-ray phase analysis (identification and quantification of phases), as well as to determine the structural characteristics of various samples in solid form, including materials based on carbon. This article summarizes the results of studies of the structural characteristics of carbon materials. Powder X-ray diffraction is used as the main method for describing the structural characteristics of crystalline ordered samples. As it turned out, carbon materials obtained on the basis of a coal tar pitch using the method of low-temperature graphitization contain simultaneously several phases of crystalline ordered carbon and amorphous carbon with a turbostructural structure. In order to explain the heterogeneous structure of carbon materials, the authors of the work compare the data of X-ray structural analysis on the main reflection reflections from the (001) plane, i.e. the most developed surface of the crystal. It was found that the (002) and (004) reflections are superpositions of components that correspond to structural phases with different interplanar distances characteristic of crystalline and amorphous carbon. From the ratio of the integrated intensities of the separated components of the reflection, the ratio between these phases is determined. The interplanar distances that characterize crystalline carbon materials were also determined, based on which the degree of order was calculated, which also makes it possible to detect the difference between the components. The degree of order, the interlayer distance (d002) and the crystalline parameters (La and Lc) are considered key parameters for the evaluation of the structure of carbon materials

References

- [1] V.I. Saranchuk, A.T. Airuni and K.E. Kovalev. Nadmolekulyarnaya organizatsiya, struktura i svoistva uglei (Supramolecular Organization, Structure, and Properties of Coals). Kiev: *Naukova Dumka*. **1988**.
- [2] A.N. Popova, S.A. Sozinov. Study of coke microstructure by combination of XRD analysis and SEM. *Butlerov Communications*. **2018**. Vol.56. No.11. P.82-89. ROI: jbc-02/18-56-11-82
- [3] Y. Cheng, Q. Zhang, Ch. Fang, Y. Ouyang, D. Liu. Co-Carbonization Behaviors of Petroleum Pitch. Waste SBS: Influence on Morphology and Structure of Resultant Cokes. *J Anal Appl Pyrol*. **2018**. No.129. P.154-164
- [4] S.A. Sozinov, L.V. Sotnikova, A.N. Popova, and R.P. Kolmikov. Study of the film of *n*-hexane insoluble asphaltene produced from coal-tar pitch. *Butlerov Communications*. **2017**. Vol.51. No.7. P.75-80. ROI: jbc-02/17-51-7-75
- [5] S.A. Sozinov, L.V. Sotnikova, A.N. Popova, L.M. Khitcova. Study of thermal decomposition product of Hexane-Insoluble Asphaltene from Coal Pitch. *Coke and Chemistry*. **2018**. Vol.61. No.11. P.47-52. (russian)
- [6] S.A. Sozinov, L.V. Sotnikova, A.N. Popova, R.P. Kolmikov, D.M. Russakov. Producing Hexane-Insoluble Asphaltene Films from Coal Pitch. *Coke and Chemistry*. **2018**. Vol.61. No.2. P.72-77. (russian)
- [7] Ch.N. Barnakov, V.Yu. Malysheva, A.N. Popova, G.P. Khokhlova, Z.R. Ismagilov. Assessment of the relationship between the structure of graphite-like materials according to the data of the Russian Federation and the electrical properties of graphite materials - anodes for LIA. *Kuzbass State Technical University Bulletin*. **2013**. No.5. P.70-73. (russian)

- [8] Ch.N. Barnakov, G.P. Khokhlova, A.N. Popova, A.I. Romanenko, Y.A. Bryantsev. Structure and conductivity of carbon materials produced from coal pitch with carbon additives. *Coke and Chemistry*. **2017**. Vol.60. No.7. P.278-284. (russian)
- [9] A.N. Popova. Crystallographic analysis of graphite by x-ray diffraction. *Coke and Chemistry*. **2017**. Vol.60. No.9. P.361-365. (russian)
- [10] Ch.N. Barnakov, G.P. Khokhlova, V.Yu. Malysheva, A.N. Popova, Z.R. Ismagilov. X-ray diffraction analysis of the crystal structures of different graphites. *Solid Fuel Chemistry*. **2015**. Vol.49. No.1. P.25-29. (russian)
- [11] A.N. Popova. The method of calculation of crystallographic characteristics of graphite. *Butlerov Communications*. **2017**. Vol.51. No.7. P.86-90. ROI: jbc-02/17-51-7-86
- [12] ICDD, PDF-2 (Database), edited by Dr. Surya Kalakkodu, International Centre for Diffraction Data. *Newtown Square, PA, USA*. **2011**.
- [13] G.P. Khokhlova, Ch.N. Barnakov, V.Yu. Malysheva, A.N. Popova, Z.R. Ismagilov. Effect of heat treatment conditions on the catalytic graphitization of coal-tar pitch. *Solid Fuel Chemistry*. **2015**. Vol.49. No.2. P.66-72. (russian)
- [14] G.P. Khokhlova, V.Yu. Malysheva, CH.N. Barnakov, A.N. Popova, Z.R. Ismagilov. Influence of the nature and amount of catalyst on the phase structure of carbon material obtained by low-temperature catalytic graphite coal tar pitch. *Kuzbass State Technical University Bulletin*. **2013**. No.5. P.21-24.
- [15] 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.
- [16] G.P. Khokhlova, C.N. Barnakov, A.N. Popova, L.M. Khitsova. Influence of carbon additives on the thermal transformation of coal pitch. *Coke and Chemistry*. **2015**. Vol.58. No.7. P.68-274. (russian)
- [17] G.P. Khokhlova, C.N. Barnakov, A.N. Popova. Carbonization of coal pitch with graphite additives. *Coke and Chemistry*. **2016**. Vol.59. No.1. P.27-34. (russian)