

Study of calcium phosphates crystallization process using the method of fractal analysis

© Vladimir M. Kiselev,¹⁺ Olga A. Golovanova,^{1*} Victor B. Fedoseev,² and Maria A. Polyntseva¹

¹ Department of Inorganic Chemistry. F.M. Dostoevsky Omsk State University.

Mira Ave., 55a. Omsk, 644077. Omsk Region. Russia. Phone: +7 (3812) 26-81-99.

E-mail: v.m.kiselev@chemomsu.ru, golovanoa2000@mail.ru

² G. A. Razuvaev Institute of Organometallic Chemistry at Russian Academy of Sciences.

Tropinin St., 49. Nizhny Novgorod, 603137. Nizhny Novgorod Region. Russia.

Phone: +7 (831) 465-61-71. E-mail: vbfedoseev@phys.unn.ru

*Supervising author; +Corresponding author

Keywords: fractal analysis, hydroxylapatite, crystallization, precipitation, calcium phosphate, fractal dimension.

Abstract

A promising direction in the field of physical chemistry is the development of methods for the study of synthetic samples based on hydroxylapatite, which is a component of human bone tissue.

With the purpose of promptly obtaining data concerning the structure and properties of the objects under study, methods with the use of the fractal analysis tool are rapidly developing in recent years. Its main advantage is the possibility of examining samples without destroying them, as well as high sensitivity, even to a slight change in properties. Potentially, the fractal analysis tool can be used to study the properties of materials based on calcium phosphates used in biomedical applications. However, there are no studies confirming this theory at the moment.

This article discusses the possibility of using the fractal analysis method for studying the crystal structures of calcium phosphates in a drying drop obtained as a result of spontaneous precipitation from an aqueous solution. Optimal deposition conditions and concentrations of solutions for this method were determined. During the study, the relationship between the fractal characteristics of the samples and the conditions of their deposition were determined (such as the concentrations of the solutions, the deposition time and the Ca/P ratio).

The paper shows that for the fractal analysis method, hydroxylapatite structures obtained by precipitation from aqueous solutions of CaCl_2 and Na_2HPO_4 with salt concentrations of 0.02-0.07 mol/l are applicable. It was found out that in the initial period of crystallization (<15 min) the fractal dimension of the hydroxylapatite structure changes insignificantly, then decreases linearly. During crystallization for several (2-5) hours a stable precipitate structure is formed, while the fractal dimension also assumes a constant value ($D = 1.2-1.25$). Obtained, the rate of decrease in the fractal dimension during the crystallization of hydroxylapatite is directly proportional to the ratio of the concentrations of Ca/P in the solution.

The resulting correlations demonstrated the high potential for using the fractal analysis method to study materials based on calcium phosphates. It can be used for the rapid evaluation of the properties of samples or for the theoretical calculation of the synthesis conditions.

References

- [1] A.G. Veresov, V.I. Putlyaev, Y.D. Tretyakov. Chemistry of inorganic biomaterials based on calcium phosphates. *Russian Journal of General Chemistry*. **2004**. Vol. XLVIII. No.4. P.32-46. (russian)
- [2] S.A. Gerk, O.A. Golovanova. Bone apatite of the person – features of a chemical structure at a pathology. *Butlerov Communications*. **2011**. Vol.24. No.3. P.123-132. ROI: jbc-02/11-24-3-123 (russian)
- [3] S.V. Dorozhkin, M. Epple. Biological and Medical Significance of Calcium Phosphates. *Angew. Chem. Int. Ed*. **2002**. Vol.41. P.3130-3146.
- [4] M.V. Berdinskaya, A.V. Zayats, O.A. Golovanova. Synthesis and research of bioresorbability of silicon-substituted hydroxylapatite. *Butlerov Communications*. **2014**. Vol.37. No.1. P.48-54. ROI: jbc-02/14-37-1-48. (russian)

- [5] O.A. Golovanova, Z.V. Romanenko. Synthesis of fluorine-containing hydroxyapatite from model solutions of the oral fluid. *Herald of Omsk University*. **2016**. No.4. P.70-74. (russian)
- [6] R.R. Izmailov, O.A. Golovanova. Solubility of hydroxyapatite and carbonate Hydroxylapatite obtained from a model solution synovial fluid of the person. *Herald of Omsk University*. **2012**. No.4. P.109-113. (russian)
- [7] I.V. Fadeeva, L.I. Shvorneva, S.M. Barinov, V.P. Orlovskiy. Synthesis and structure of magnesium substituted hydroxyapatite. *Inorganic Materials*. **2003**. Vol.39. No.9. P.1102-1105. (russian)
- [8] A.P. Solonenko, O.A. Golovanova, M.V. Filchenko and others. Physico-chemical investigation of the «hydroxyapatite – brushite» compositions, received by co-precipitation. *Herald of Omsk University*. **2012**. No.2. P.135-142. (russian)
- [9] V.V. Smirnov, M.A. Goldberg, L.I. Shvorneva and others. Synthesis of composite biomaterials in the hydroxyapatite-calcite system. *Doklady Chemistry*. **2010**. Vol.432. No.2. P.199-202. (russian)
- [10] W. Suchanek, M. Yoshimura. Processing and properties of HA-Based biomaterials for use as hard tissue replacement implants. *J. Mater. Res. Soc.* **1998**. Vol.13. No.1. P.94-103.
- [11] A.V. Kuznetsov, A.S. Fomin, A.G. Veresov and others. Hydroxyapatite of platelet morphology synthesized by ultrasonic precipitation from solution. *Russian Journal of Inorganic Chemistry*. **2008**. Vol.53. No.1. P.5-10. (russian)
- [12] S.V. Panin, O.V. Startsev, A.S. Krotov and others. Corrosion and aging of structural materials according to 3D microscopy. Proceedings of VIAM. **2014**. No.12. URL: http://www.viam-works.ru/ru/articles?art_id=756dx.doi.org/10/18577/2307-6046-2014-0-12-12-12 (russian)
- [13] V.M. Kiselev, O.A. Golovanova, V.B. Fedoseev, T.S. Gryaznova. The using of fractal analysis methods in studying of titanium alloy VT1-0. *Herald of Omsk University*. **2016**. No.2. P.44-49. (russian)
- [14] E.N. Fedoseeva, V.B. Fedoseev. Interaction of chitosan with benzoic acid in solution and films. *Polymer Science, Ser. A*. **2011**. Vol.53. No.11. P.1900-1907. (russian)
- [15] A. Kh. Malamatov. Theoretical description of high-density polyethylene crystallization in the framework of fractal analysis. *Modern High Technologies*. **2005**. No.11. P.58-59. (russian)
- [16] S.M. Barinov, V.S. Komlev. Bioceramics based on calcium phosphates. *Moscow: Nauka*. **2005**. 204p. (russian)
- [17] A.P. Solonenko, O.A. Golovanova, V.S. Ishutina. Determination of the possibility and conditions of brushite deposition from aqueous solutions under varying the parameters of the crystallization medium. *Butlerov Communications*. **2010**. Vol.21. No.8. P.17-27. ROI: jbc-02/10-21-8-17
- [18] A.P. Solonenko, O.A. Golovanova. Thermodynamic modeling of calcium orthophosphates formation. *Butlerov Communications*. **2011**. Vol.24. No.2. P.106-112. ROI: jbc-02/11-24-2-106
- [19] V.U. Yelnikov, E.V. Rosseeva, O.A. Golovanova, O.V. Frank-Kamenetskaya. Thermodynamic and experimental modeling of the formation of the main mineral phases of kidney stones. *Russian Journal of Inorganic Chemistry*. **2007**. Vol.52. No.2. P.190-197. (russian)
- [20] *Patent 2546539 (Rus)*, A61L27/12, A61L27/32, C04B35/447, C01B25/32. Method for producing a powder material based on carbonate hydroxyapatite and brushite. Solonenko A.P., O.A. Golovanova. F.M. Dostoevsky Omsk State University. Publ. 10.04.2015. (russian)
- [21] O.A. Golovanova, A.A Solodyankina. Crystallization of calcium phosphates from solutions simulating the composition of human blood plasma. *Butlerov Communications*. **2013**. Vol.36. No.11. P.104-110. ROI: jbc-02/13-36-11-104