fractal and fractional

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Editorial

Fractal Analysis and Fractal Dimension in Materials Chemistry

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1. Introduction

Using fractal analysis and computing fractal dimension to understand materials chemistry and solve problems such as catalysis, chemical reactions, fuel storage, and material design is an important scientific research domain. After B. B. Mandelbrot [1,2] published his works regarding fractals, defining them as objects with a peculiar geometry and characterized by fractional exponents, it seemed that fractal theory would be the answer to questions in different domains: engineering, physics and chemistry, computer science, even literature and geography. After Avnir, Farin, and Pfeifer [3] found that surfaces of most materials are fractals at molecular scale, studies intensified in the following directions: fractal dimension determination of materials by micrograph analysis [4–8], adsorption isotherms method [9–13], small-angle X-Ray scattering [14], relation between physical and chemical properties of materials and the fractal dimension to design better materials [15,16], application of fractal analysis on adsorption, chemisorption, chemical reactions, heterogeneous catalysis [17–29], medicine and cancer research [30,31].

Scientific literature related to fractal analysis in materials chemistry depicts two essential research fields: first, characterization of materials from the fractal point of view to find self-similarity in nature and second, to correlate experimental conditions and preparation routes with the fractal behavior to design specific materials. The articles published in this special issue are part of these scientific research directions and state-of-the-art applications of fractal theory in materials chemistry.

Seven articles were successfully published following the excellent collaboration with Ms. Assistant Editor May Mei and the editing team's special work. Finally, we are grateful to all the authors of these publications for their excellent research work and contribution to this Special Issue.

2. This Special Issue

Qi An et al. in Contribution 1 have developed a novel analytical model based on the Sierpinski carpet to obtain the normal contact stiffness on the grinding joint surface. The model was compared with the KE model and experimental data, and the presented model was found to be close to experimental data. It was proved that the model is a solid theoretical base for the optimization design of high-precision machine tools. The relation between design and the fractal analysis is underlined.

In Contribution 2, Z. D. Ghizdavet et al. obtained alumina ceramics from different alumina sources using various rare-earth dopants, concentration levels, and synthesizing routes. A total of 206 Scanning Electron Microscopy micrographs were compared using fractal theory. Fractal dimension was used to mark dissimilar or noisy micrographs and identify correlations. Using different fractal dimension determination methods, two edge detection techniques, ImageJ's Find Edges tool, and the Canny Edge Detection plugin also led to selecting the best method in terms of processing time and quality: the Canny Edge Detection plugin. This paper's strong dependence on synthesizing conditions and similarities is an important finding.

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G. Dobrescu et al. (Contribution 3) found the well-known Dubinin-Radushkevitch and fractal Freundlich isotherms using Cerofolini's model and an adequate adsorption energy form. The surfaces' energetic and geometric properties are assumed to exhibit fractal behavior. This theoretical approach explains why the sorbent does not need to be porous to apply a fractal adsorption isotherm and offers interesting insights on fractal energetic inhomogeneities behavior. The theory was applied to some nanoparticle catalysts (Rh/Al_2O_3, Rh/TiO_2, and Rh/WO_3), and some experimental results were discussed from this point of view.

In Contribution 4, Shansi Tian et al. choose to analyze the microstructure of pores and to characterize the multifractal behavior of the heterogeneity of the pores of a natural lacustrine oil-prone shale. FE-SEM micrographs were used to describe the pores fractality of the four pore types: organic pores, organic cracks, inorganic pores, and inorganic cracks. Their principal findings reside that the inorganic pores and cracks are the main storage space; organic pores and cracks provide only limited resources.

Gabriela Petcu et al. in Contribution 5 analyze in situ morphology, structure, and fractal dimension during the zeolitization of Zeolite Y and Ti-containing zeolite Y. Fractal dimensions were computed from small-angle X-ray scattering (SAXS): transition from small particles with a smooth surface to compact structures of zeolite crystallites with rough surfaces was depicted from fractal dimension variation. Titanium incorporation in low concentration into the zeolite Y leads to smooth surfaces and compact structures with lower fractal dimensions; meanwhile, higher Ti concentration leads to higher fractal dimensions and higher self-similarity properties. These observations lead to a mechanism to describe the zeolite synthesis.

In Contribution 6, authors Cheng Li et al., a fractal pore-scale model is used to study the fluid flow, heat conduction, and gas diffusion through porous media. They also calculate the conductivity properties, such as effective permeability, thermal conductivity, and diffusion coefficient. Results depicted the correlations between conductivity and the pore structure. Experimental results and 2D numerical simulations were compared with the theoretical findings, providing new insights for understanding the transport processes through porous materials. Results could solve problems such as energy storage, carbon dioxide sequestration, fuel cells, etc.

The authors F.M. Mwema et al. in Contribution 7 bring an interesting approach to the growing trend in research on the applications of fractal theory in thin film technology. The bibliometric study also discussed the factors that influenced this behavior. Authors identified four application domains: (1) fractal theory as a tool for the creation of superior devices, (2) using fractal theory for characterization of roughness and structure evolution, (3) using fractal theory for prediction of structure evolution during thin film depositions and (4) fractal theory as an optimization tool for thin film design.

In conclusion, this Special Issue, "Fractal Analysis and Fractal Dimension in Materials Chemistry", is a collection of papers dedicated to studying the fractal properties of materials in their preparation and characterization phases. From this point of view, this issue is a useful tool for researchers interested in fractal dimension determination by micrograph image analysis (SEM) or SAXS, adsorption isotherms and characterization of surface energetic inhomogeneities, materials and high-precision machine tools design, porous materials, and finally, thin films.

Conflicts of Interest: The authors declare no conflict of interest.

List of Contributions

1. An, Q.; Liu, Y.; Huang, M.; Suo, S. A Novel Contact Stiffness Model for Grinding Joint Surface Based on the Generalized Ubiquitiformal Sierpinski Carpet Theory. *Fractal Fract.* **2024**, *8*, 351. https://doi.org/10.3390/fractalfract8060351.

2. Ghizdavet, Z.D.; Volceanov, A.; Volceanov, E. Multivariate Analysis on a Complex, Rare-Earth Doped Alumina Database with Fractal Dimension as a Microstructural Quantifier. *Fractal Fract.* **2023**, *7*, 286. https://doi.org/10.3390/fractalfract7040286.
3. Dobrescu, G.; Papa, F.; Culita, D.; Balint, I.; Ionescu, N.I. Cerofolini's Model and the Fractal Adsorption Isotherms. *Fractal Fract.* **2023**, *7*, 262. https://doi.org/10.3390/fractalfract7030262.
4. Tian, S.; Guo, Y.; Dong, Z.; Li, Z. Pore Microstructure and Multifractal Characterization of Lacustrine Oil-Prone Shale Using High-Resolution SEM: A Case Sample from Natural Qingshankou Shale. *Fractal Fract.* **2022**, *6*, 675. https://doi.org/10.3390/fractalfract6110675.
5. Petcu, G.; Dobrescu, G.; Atkinson, I.; Ciobanu, M.; Blin, J.-L.; Parvulescu, V. Evolution of Morphology, Fractal Dimensions, and Structure of (Titanium) Aluminosilicate Gel during Synthesis of Zeolites Y and Ti-Y. *Fractal Fract.* **2022**, *6*, 663. https://doi.org/10.3390/fractalfract6110663.
6. Li, C.; Xu, Y.; Jiang, Z.; Yu, B.; Xu, P. Fractal Analysis on the Mapping Relationship of Conductivity Properties in Porous Material. *Fractal Fract.* **2022**, *6*, 527. https://doi.org/10.3390/fractalfract6090527.
7. Mwema, F.M.; Jen, T.-C.; Kaspar, P. Fractal Theory in Thin Films: Literature Review and Bibliometric Evidence on Applications and Trends. *Fractal Fract.* **2022**, *6*, 489. https://doi.org/10.3390/fractalfract6090489.

References

1. Mandelbrot, B.B. *Fractals: Form, Chance and Dimension*; Freeman, W.H., Ed.; MANDELBROT. WH Freeman and Co.: San Francisco, CA, USA, 1977.
2. Mandelbrot, B.B. *The Fractal Geometry of Nature*; Freeman, W.H., Ed.; MANDELBROT. WH Freeman and Co.: San Francisco, CA, USA, 1982.
3. Avnir, D.; Farin, D.; Pfeifer, P. Surface geometric irregularity of particulate materials: The fractal approach. *J. Colloid Interface Sci.* **1985**, *103*, 112–123. [CrossRef]
4. Miyazaki, A.; Matsuda, K.; Papa, F.; Scurtu, M.; Negrila, C.; Dobrescu, G.; Balint, I. Impact of particle size and metal-support interaction on denitration behavior of wee-defined Pt-Cu nanoparticles. *Catal. Sci. Technol.* **2015**, *5*, 492–503. [CrossRef]
5. Schepers, H.E.; van Beek, J.H.G.M.; Bassingthwaighte, J.B. Four methods to estimate the fractal dimension from self-affine signals (medical application). *IEEE Eng. Med. Biol.* **1992**, *11*, 57–64. [CrossRef]
6. Botet, R.; Jullien, R. A theory of aggregating systems of particles: The clustering of clusters process. *Ann. Phys. Fr.* **1988**, *13*, 153–221. [CrossRef]
7. Family, F.; Vicsek, T. Scaling of the active zone in the Eden process on percolation networks and the ballistic deposition model. *J. Phys. A Math. Gen.* **1985**, *18*, L75–L81. [CrossRef]
8. Chauvy, P.F.; Madore, C.; Landolt, D. Variable length scale analysis of surface topography: Characterization of titanium surfaces for biomedical applications. *Surf. Coat. Technol.* **1998**, *110*, 48–56. [CrossRef]
9. Cole, M.W.; Holter, N.S.; Pfeifer, P. Henry's law of adsorption on a fractal surface. *Phys. Rev. B* **1986**, *33*, 8806–8809. [CrossRef]
10. Fripiat, I.J.; Gatineau, L.; van Damme, H. Multilayer physical adsorption on fractal surface. *Langmuir* **1986**, *2*, 562–567. [CrossRef]
11. Pfeifer, P.; Obert, M.; Cole, M.W. Fractal BET and FHH Theories of Adsorption: A Comparative Study. *Proc. R. Soc. Lond. A* **1989**, *423*, 169–188. [CrossRef]
12. Pfeifer, P.; Wu, Y.J.; Cole, M.W.; Krim, J. Multilayer adsorption on a fractally rough surface. *Phys. Rev. Lett.* **1989**, *62*, 1997–2000. [CrossRef]
13. Avnir, D.; Jaroniec, M. An isotherm equation for adsorption on fractal surfaces of heterogeneous porous materials. *Langmuir* **1989**, *5*, 1431–1433. [CrossRef]
14. de Moor, P.-P.E.A.; Beelen, T.P.M.; Komanschek, B.U.; Diat, O.; van Santen, R.A. In Situ Investigation of Si-TPA-MFI Crystallization Using (Ultra-) Small- and Wide-Angle X-ray Scattering. *J. Phys. Chem. B* **1997**, *101*, 11077–11086. [CrossRef]
15. Trypolskyi, A.I.; Gurnyk, T.M.; Strizhak, P.E. Fractal dimension of zirconia nanopowders and their activity in the CO oxidation. *Catal. Commun.* **2011**, *12*, 766–771. [CrossRef]
16. Papa, F.; Berger, D.; Dobrescu, G.; State, R.; Ionescu, N.I. Correlation of the Sr-dopant content in $La_{1-x}Sr_xCoO_3$ with catalytic activity for hydrogen peroxide decomposition. *Rev. Roum. Chim.* **2018**, *63*, 447–453.
17. Rothschild, W.G. Fractals in heterogeneous catalysis. *Catal. Rev. Sci. Eng.* **1991**, *33*, 71–107. [CrossRef]
18. Pfeifer, P.; Avnir, D.; Farin, D. Complex Surface Geometry in Nano-Structure Solids: Fractal Versus Bernal-Type Models. In *Large Scale Molecular Systems—Quantum and Stochastic Aspects*; Gans, W., Blumen, A., Amann, A., Eds.; NATO ASI, Series B; Plenum: New York, NY, USA, 1991; pp. 215–229.

19. Meakin, P. Fractals and Reactions on Fractals. In *Reactions in Compartmentalized Liquids*; Knoche, W., Schomäcker, R., Eds.; Springer: Berlin/Heidelberg, Germany, 1989; pp. 173–198.
20. Pfeifer, P.; Kenntner, J.; Cole, M.W. Detecting capillary condensation in the absence of adsorption/desorption hysteresis. In *Fundamentals of Adsorption*; American Institute of Chemical Engineers: New York, NY, USA, 1991; pp. 689–700.
21. Ludlow, D.K.; Moberg, T.P. Technique for determination of surface fractal dimension using a dynamic flow adsorption instrument. *Instrum. Sci. Technol.* **1990**, *19*, 113–123. [CrossRef]
22. Farin, D.; Avnir, D.; Pfeifer, P. Fractal dimensions of surfaces. The use of adsorption data for the quantitative evaluation of geometric irregularity. *Particul. Sci. Technol.* **1984**, *2*, 27–35. [CrossRef]
23. Pfeifer, P.; Stella, A.L.; Toigo, F.; Cole, M.W. Scaling of the dynamic structure factor of an adsorbate on a fractal surface. *Europhys. Lett.* **1987**, *3*, 717–722. [CrossRef]
24. Cheng, E.; Cole, M.W.; Pfeifer, P. Defractalization of films adsorbed on fractal surfaces. *Phys. Rev. B* **1989**, *39*, 12962–12965. [CrossRef]
25. Avnir, D.; Farin, D. Fractal scaling laws in heterogeneous chemistry: Part I: Adsorptions, chemisorptions and interactions between adsorbates. *New J. Chem.* **1990**, *14*, 197–206.
26. Pfeifer, P.; Johnston, G.P.; Deshpande, R.; Smith, D.M.; Hurd, A.J. Structure analysis of porous solids from preadsorbed films. *Langmuir* **1991**, *7*, 2833–2843. [CrossRef]
27. Kaneko, K.; Sato, M.; Suzuki, T.; Fujiwara, Y.; Nishikawa, K.; Jaroniec, M. Surface fractal dimension of microporous carbon fibres by nitrogen adsorption. *J. Chem. Soc. Faraday Trans.* **1991**, *87*, 179–184. [CrossRef]
28. Gutfraind, R.; Sheintuch, M.; Avnir, D. Fractal and multifractal analysis of the sensitivity of catalytic reactions to catalyst structure. *J. Chem. Phys.* **1991**, *95*, 6100–6111. [CrossRef]
29. Sanders, L.M.; Ghaisas, S.V. Fractals and patterns in catalysis. *Phys. A* **1996**, *233*, 629–639. [CrossRef]
30. Metze, K. Fractal dimension of chromatin: Potential molecular diagnostic applications for cancer prognosis. *Expert Rev. Mol. Diagn.* **2013**, *13*, 719–735. [CrossRef]
31. Contaldo, M.; Di Spirito, F.; Di Palo, M.P.; Amato, A.; Fiori, F.; Serpico, R. Fractal Analysis Applied to the Diagnosis of Oral Cancer and Oral Potentially Malignant Disorders: A Comprehensive Review. *Appl. Sci.* **2024**, *14*, 777. [CrossRef]