Dr. Yuri Georgievich Chirkov

Dr. Yuri Georgievich Chirkov is Senior Researcher at the Frumkin Institute of Electrochemistry (Leninskii pr.31, Moscow, 117071 Russia), affiliated with the Russian Academy of Science. Dr. Chirkov is an active member of the Russian Federation Academy of Medical and Technical Sciences.

Dr. Chirkov's main research interests are in the field of theory of porous electrodes (fuel cells, electrolysis, rechargeable batteries, etc). Dr. Chirkov has authored over 300 research papers, including:

- chapters in *Macrokinetics of Processes in Porous Media (Makrokinetika protsessov v poristykh sredakh),* by Chizmadzhev Yu.A., Markin V.S., Tarasevich M.R., and Chirkov Yu.G.; Moscow: Nauka, 1971, and
- chapter in *Comprehensive Treatise of Electrochemistry,* Plenum Press, Vol. 6, pp.317-391, 1983.

Dr. Chirkov has worked on the following projects:

<u>1. Percolation.</u>

Relevant publication:

Theory of Porous Electrodes: The Percolation and a Calculation of Percolation Lines (in the Russian Journal of Electrochemistry, vol. 35, no. 12, 1999, pp. 1281-1290).

<u>2. Computer Simulation and Calculating Overall Electrochemical Characteristics of Cathode for Polymer Electrolyte Membrane Fuel Cells (PEMFC).</u>

Relevant publications:

- Chirkov Yu.G., Rostokin V.I. Optimizing Weights of Platinum in the Active Layer of the Cathode of a Hydrogen-Oxygen Fuel Cell with a Solid Polymer Electrolyte. Russian Journal of Electrochemistry. 2004. V.40. No.9. pp.898-908.
- Chirkov Yu.G., Rostokin V.I. Cathode of a Hydrogen-Oxygen Fuel Cell with a Solid Polymer Electrolyte: The Effect of the Flooding of Pores by Water on the Characteristics of the Active Layer. Russian Journal of Electrochemistry. 2005. V.41. No.1. pp. 32-43.
- Chirkov Yu.G., Rostokin V.I. Calculating a Characteristic Bulk Current Density in the Cathode of a Hydrogen-Oxygen Fuel Cell with a Solid Polymer Electrolyte. Russian Journal of Electrochemistry. 2005. V.41. No.9. pp. 985-995.
- Chirkov Yu.G., Rostokin V.I. Active Layer of the Cathode of a Fuel Cell with a Solid Polymer Electrolyte: The Effect of the Nafion Concentration on the Overall Characteristics. Russian Journal of Electrochemistry. 2006. V.42. No.7. pp. 799-805.
- Chirkov Yu.G., Rostokin V.I. Theory of Porous Electrodes: Calculation of Overall Cathode Characteristics for the Case Where the Polarization Curve Has Segments with Different Slopes. Russian Journal of Electrochemistry. 2006. V.42. No.7. pp. 806-812.
- Chirkov Yu.G., Rostokin V.I. Calculation of the Liquid and Gas Permeability of Hydrophobic Low-Porosity Membranes of an Arbitrary Thickness. Russian Journal of Electrochemistry. 2004. V.40. No.2. pp.158-169.

- Chirkov Yu.G., Rostokin V.I. Cathode of a Fuel Cell with a Solid Polymer Electrolyte: Calculating Overall Currents in the Presence of a Gas-Diffusion Layer. Russian Journal of Electrochemistry. 2007. V.43. No. 1, pp.25-33.
- Chirkov Yu.G., Rostokin V.I. «Fuel Cell Cathode with Nafion and Platinum: Calculating its Overall Performance with Consideration of Gas- and Vapor-Exchange Processes in the Gas-Diffusion Layer» // Russ. J. Electrochem. 2008. V. 44. P. 910-920.
- Chirkov Yu.G., Rostokin V.I. «Hydrogen–Oxygen (Air) Fuel Cell with Nafion and Platinum: Calculating Overall Characteristics, Comparing the Performance of a Cathode with Polymeric Electrolyte with a Hydrophobized Cathode with Liquid Electrolyte» // Russian Journal of Electrochemistry, 2008, Vol. 44, No. 11, pp. 1228–1239.
- Chirkov Yu.G., Rostokin V.I. «Calculation of Optimum Thickness of Active Layer of Oxygen and Air Cathodes of Fuel Cell with Nafion and Platinum» // Russian Journal of Electrochemistry, 2009, Vol. 45, No. 2, pp. 183–191.

- Chirkov Yu.G., Rostokin V.I. «Fuel Cell Oxygen Cathode with Nafion and Platinum: the Effect of Active Layer Heating on Overall Cathode Characteristics» // Russ. J. Electrochem. 2009. V. 45. P. 1027-1036.
- Chirkov Yu.G., Rostokin V.I. «Fuel Cell with Polymer Electrolyte: Calculation of Overall Characteristics of Oxygen Cathode with Account for Processes of Gas, Vapor, and Heat Exchange» // Russ. J. Electrochem. 2009. V. 45. P. 1253-1265.
- Chirkov Yu.G., Rostokin V.I. «Active Layer of an Electrode with Polymer Electrolyte: Estimation of Platinum Utilization Degree» // Russian Journal of Electrochemistry, 2009, Vol. 45, No. 12, pp. 1376–1386.
- Yu. G. Chirkov, M. P. Tarasevich, and V. M. Andoralov «Polymer Electrolyte Fuel Cell: Comparison of Dimensional Specifications of Cathodes with Platinum and Palladium Based Catalysts» // Russian Journal of Physical Chemistry A, 2010, Vol. 84, No. 1, pp. 98–103.
- Chirkov Yu.G., Rostokin V.I. «Активный слой катода топливного элемента с полимерным электролитом: модель комбинированных зерен, расчет габаритных характеристик» // Russ. J. Electrochem. 2011. V. 47. P. 59-70.
- Chirkov Yu.G., Rostokin V.I. «Компьютерное моделирование активного слоя катода топливного элемента с полимерным электролитом: формирование полноценных зерен углеродной подложки, расчет габаритных характеристик» // Альтернативная энергетика и экология. 2012, №2, С.132-145.
- Chirkov Yu.G., Rostokin V.I. «Active Layer of Fuel Cell Electrode with Polymer Electrolyte: Nature of Proton and Oxygen Supply Channels» // Russ. J. Electrochem. 2012. V. 48. P. 1086-1096.
- Chirkov Yu.G., Rostokin V.I. «Active Layer of Fuel Cell Electrode with Polymer Electrolyte: Modeling of Support Grains, Calculation of Overall Cathode Characteristics » // Russ. J. Electrochem. 2013. V. 49. P. 149-160.
- Chirkov Yu.G., Rostokin V.I. «Computer Simulation of Active Layer of Fuel Cell Electrode with Polymer Electrolyte: Complete Combined Carbon Support Grains, Calculation of Overall Characteristics» // Russ. J. Electrochem. 2013. V. 49. P.428-440.

3. Computer Simulation and Calculating Overall Electrochemical Characteristics of Cathode for Phosphoric Acid Electrolyte Fuel Cells (PAFC).

Relevant publication:

- Chirkov Yu.G., Rostokin V.I. Hydrophobized Oxygen Cathode of a Fuel Cell with a Liquid Electrolyte: Calculating Overall Currents and Thicknesses. Russian Journal of Electrochemistry. 2007. V.43. No. 2, pp.146-156.

4. Computer Simulation of Porous Electrodes with Immobilized Enzymes.

Relevant publications:

- Chirkov Yu.G., Rostokin V.I. Computer Simulation of Porous Electrodes with Immobilized Enzymes: The Percolation Properties of Multicomponent Structures. Russian Journal of Electrochemistry. 2002. V.38. No.9. pp.1016-1024.
- Chirkov Yu.G., Rostokin V.I. Computer-Aided Simulation of Porous Electrodes of a Filled-up Type. Russian Journal of Electrochemistry. 2003. V.39. No.6. pp.622-631.
- Chirkov Yu.G., Rostokin V.I. Calculating the Electrochemical Activity of Porous Electrodes of a Filled-up Type with an Immobilized Enzyme. Russian Journal of Electrochemistry. 2003. V.39. No.6. pp. 632-641.
- Chirkov Yu.G., Rostokin V.I. Calculating Electrochemical Activity of Porous Electrodes of a Filled-up Type with an Immobilized Enzyme and Regular Gas Pores. Russian Journal of Electrochemistry. 2003. V.39. No.7. pp.731-742.
- Chirkov Yu.G., Rostokin V.I. Computer-aided Modeling of Porous Electrodes with an Immobilized Enzyme: Substrates with a Partially Regular Structure. Russian Journal of Electrochemistry. 2003. V.39. No.12. pp.1321-1330.
- Chirkov Yu.G., Rostokin V.I. Calculating Electrochemical Activity of Regular-Structure Porous Electrodes with an Immobilized Enzyme. Russian Journal of Electrochemistry. 2004. V.40. No.1. pp.27-35.
- Chirkov Yu.G., Rostokin V.I. Porous Electrodes with Immobilized Enzymes: The Fractal-Percolation Properties of Supports Manufactured from Particles of Finely Divided Colloidal Graphite. Russian Journal of Electrochemistry. 2005. V.41(8). pp.838-848.
- Chirkov Yu.G., Rostokin V.I. Porous Electrodes with an Immobilized Enzyme: The Problem of Development of Nanocomposites with High Concentrations of Molecules of Active Enzymes. Russian Journal of Electrochemistry. 2005. V.41(11). pp. 1221-1230.
- Chirkov Yu.G., Rostokin V.I. Computer Simulation of the Structure of Porous Electrodes with an Immobilized Enzyme and Nanosized Support Particles. Russian Journal of Electrochemistry. 2005. V.41(6).
- Tarasevich M.R., Chirkov Yu.G., Bogdanovskaya V.A., Kapustin A.V. Fractal and percolation properties of active layer structure at oxygen electrode based on nanocomposite material of dispersed carbon carrier/laccase. Electrochimica Acta 51 (2005) 418-426.

5. Theory of Gas-Generating Porous Electrodes.

What has been done:

(i) General theory, in region overvoltage from zero to maximum possible, of gas-generating porous electrodes (GPE) was created.

(ii) Decisive influence porous structure of GPE upon electrochemical characteristics was proved.

(iii) Concrete example of GPE, DSA, chlorine electrolysis, was studied. Calculated are: the polarization curves, the effective penetration depth of the electrochemical gas generation process in porous electrode, standard thickness active layer of electrode and so on. The predictions of the theory against what was observed in real DSA was set.

DSA (chlorine electrolysis):

The structure of the porous space of DSA that are employed in the chlorine electrolysis, the existence of micropores and macropores in these electrodes have come to life spontaneously, this structure is a side effect of the state-of-the-art technology of DSA fabrication. No one has ever tried to control parameters of DSA. By doing this, one could hope to considerable improve electrochemical characteristics of DSA. Then one would have managed to reduce the working overvoltage and diminish ohmic restrictions, and these, according to calculations, are principal barriers that do not allow one to improve electrochemical characteristics of DSA. It may hope, according to calculations, to increase size of electrochemical activity of DSA twice (100%). But only cooperation of efforts theory and technology can create new generation of DSA.

Theory must receive optimized characteristics of DSA (chlorine electrolysis). This work will have the following stages:

1. Computer porous structure simulation of DSA.

2. Calculating basic electrochemical characteristic of such models of DSA.

3. Search, this is final intention, optimum parameters of porous structure, optimal variants of DSA, with maximum of electrochemical activity.

Relevant publications:

- Chirkov Yu.G., Chernenko A.A. Gas-generating Porous Electrodes: The Nature of the Low-Polarizability Portion in the Polarization Curves Russ. J. of Electrochem. 2001. V.37. No.5. pp.467-476.
- Chirkov Yu.G., Rostokin V.I. Gas-generating Porous Electrodes: Calculating Characteristics in the Low-Polarizability Portion Russ. J. of Electrochem. 2001. V.37. No.5. pp.477-485.
- Chirkov Yu.G., Rostokin V.I. Gas-generating Porous Electrodes: Allowing for the Ohmic Limitations Russ. J. of Electrochem. 2001. V.37. No.8. pp.848-856.
- Chirkov Yu.G., Rostokin V.I. Gas-generating Porous Electrodes: Large Ohmic Resistances Russ. J. of Electrochem. 2001. V.37. No.9. pp.952-959.
- Chirkov Yu.G., Rostokin V.I. Gas-generating Porous Electrodes: Why Is Ii that the "Standard" Thickness of DSA (Chlorine Generation) Equals Five Micrometers? Russ. J. of Electrochem. 2002. V.38. No.3. pp.280-284.
- Chirkov Yu.G., Rostokin V.I. Gas-generating Porous Electrodes: Effect of the Catalyst Activity on the Polarization Curves. Russian Journal of Electrochemistry. Russ. J. of Electrochem. 2002. V.38. No.3. pp.285-292.

<u>6. Computer Simulation of Negative and Positive Electrodes in Lithium-Ion Battery\</u>

Relevant publications:

- Chirkov Yu.G., Rostokin V.I., Skundin A.M. «Computer Modeling of Negative Electrode Operation in Lithium–Ion Battery: Model of Equal–Sized Grains, Galvanostatic Discharge Mode, Calculation of Characteristic Parameters» // Russ. J. Electrochem. 2011. V. 47. P. 59-70.
- Chirkov Yu.G., Rostokin V.I., Skundin A.M. «Computer Modeling of Positive Electrode Operation in Lithium–Ion Battery: Model of Equal–Sized Grains, Percolation Calculations» // Russ. J. Electrochem. 2011. V. 47. P. 71-83.
- Chirkov Yu.G., Rostokin V.I., Skundin A.M. «Computer Simulation of Negative Electrode Operation in Lithium–Ion Battery: Galvanostatic Discharge, Active Intercalating Agent Grains, Role of Diffusion Limitations» // Russ. J. Electrochem. 2011. V. 47. P. 288-298.
- Chirkov Yu.G., Rostokin V.I., Skundin A.M. «Computer Simulation of Negative Electrode Operation in Lithium–Ion Battery: Galvanostatic Discharge, Porous Electrode Model and Film Model» // Russ. J. Electrochem. 2011. V. 47. P. 299-309.
- Chirkov Yu.G., Rostokin V.I., Skundin A.M. «Computer Simulation of the Negative Electrode Operation in Lithium Ion Battery: Galvanostatics, the Problem of Calculating Working Parameters» // Russ. J. Electrochem. 2011. V. 47. P. 768-780.
- Chirkov Yu.G., Rostokin V.I., Skundin A.M. «Computer Simulation of Operation of Lithium-Ion Battery: Galvanostatics, Central Problem of Theory, Calculation of Characteristics of Thin Active Layers with Low Diffusion Coefficients» // Russ. J. Electrochem. 2011. V. 47. P. 1239-1249.
- Chirkov Yu.G., Rostokin V.I., Skundin A.M. «Computer Simulation of Negative Electrode Operation in Lithium-Ion Battery: Optimization of Active Mass Composition» // Russ. J. Electrochem. 2012. V. 48. P. 895-904.
- Chirkov Yu.G., Rostokin V.I., Skundin A.M. « Литий-ионный аккумулятор, гальваностатический режим разряда: расчет рабочих параметров анода с высокими и низкими значениями коэффициента диффузии атомов лития» // Alternative energy and ecology. 2012, №9, С.142-151.
- Chirkov Yu.G., Rostokin V.I., Skundin A.M. «Lithium Ion Rechargeable Battery, Galvanostatics: Computer Simulation and Calculation of Characteristics of the Anode Active Layer of Arbitrary Thickness with Low Lithium Diffusivity» // Russ. J. Electrochem. 2013. V. 49. P.545-556.