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FEATURES OF ION EXCHANGE BETWEEN THE ELECTRODES IN METAL-ION BATTERIES DURING DISCHARGE

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The importance and relevance of the storage of electrical energy is confirmed by events in the world and trends in the development and use of various electrical energy systems, household appliances, computer equipment, communication devices, etc. In addition to the growth of the metal-ion battery markets, there are trends towards a search for metals that in the future will be inexpensive and will have characteristics required for storage systems.

This paper considers ion exchange between the electrodes of metal-ion batteries whose charge carriers are metal ions, which diffuse in the process of discharge from the negative electrode to the positive one. A mathematical model was developed and tested. The model is based on a system of diffusion transport equations with the Nernst–Planck–Poisson potential equation replaced by an equivalent conductivity potential equation. Quasi-equilibrium regimes are considered.

The entire working area consists of a pore electrode space and a neutral separator. The mathematical model employed consists of potential distribution equations and an electrolyte concentration distribution equation supplemented by the dependence of the electrode surface current on the overvoltage and equations that determine the electrode pore structure depending on the masses transferred inside the electrode.

The electric potential and diffuse component mass transfer equations are written within the framework of the modern theory of effective electrical conductivity in batteries with account for current exchange between the solid electrodes and the liquid electrolyte.

The research results showed the following. A change in the resistance of the separator (a change in porosity) has little effect, if any, on the electrode current densities, but it causes some change in the potentials themselves. A change in the resistance of the electrolyte affects both the electrode potentials and the internal current distribution between the electrodes and the electrolyte.

Keywords: *metal-ion battery, separator, anode, cathode, system of equations, porosity, potential, diffusion transport*.

1. Verma J., Kumar D. Metal-ion batteries for electric vehicles: current state of the technology, issues and future perspective. Nanoscale Adv. 2021, V. 3. No. 12. Pp. 3384-3394.
https://doi.org/10.1039/D1NA00214G

2.Koshel M. D. Theoretical Foundations of Electrochemical Energetics. Dnipropetrovsk: UDKhTU, 2002. 430 pp. (in Ukrainian).

3. Byk M. V., Frolenkova S. V., Buket O. I., Vasylev H. S. Engineering Electrochemistry. Part 2. Chemical Current Sources. Kyiv: KPI, 2018. 321 pp. (in Ukrainian).

4. Ramos A. M. On the well-posedness of a mathematical model for lithium-ion batteries Applied Mathematical Modelling. 2016. V. 40. Pp. 115-125.
https://doi.org/10.1016/j.apm.2015.05.006

5. Binelo M. F. B., Sausen A. T. Z. R., Sausen P. S., Binelo M. O. Mathematical modeling and parameter estimation of battery lifetime
using a combined electrical model and a genetic algorithm. Tend. Mat. Apl. Comput. 2019. V. 20. No. 1. Pp. 150- 167.
https://doi.org/10.5540/tema.2019.020.01.149

6. Borakhadikar Ashwin S. One Dimensional Computer Modeling of a Lithium-Ion Battery A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Mechanical Engineering. Shivaji University, Kolhapur, 2013. 71 pp.

7. Esfahanian Vahid, Torabi Farschad, Mosahebi Ali . An improved mathematical model of lead-acid batteries for simulation of VRLA batteries. Journal of Power Sources Symposium. 2007. 9 pp. URL:
https://wp.kntu.ac.ir/ftorabi/Resources/Publications/An%20Improved%20Mathematical%20Model%20of%20Lead%E2%80%93Acid%20Batteries%20for%20Simulation%20of%20VRLA%20Batteries.pdf (Last accessed on April 28, 2023).

8. Esfahanian Vahid, Kheirhan Pooyan, Bahramian Hassan, Ansori Amir Babac, Ahmadi Goodarz. The effects of electrode parameters on lead-acid battery performance. Advanced Materials Research. 2013. V. 651. Pp. 492 -498. https://doi.org/10.4028/www.scientific.net/AMR.651.492

9. Gu Hiram, Nguyen T. V., White R.E. A mathematical model of a lead-acid cell: discharge, rest, and charge. J. Electrochem. Soc. Electrochemical Science and Technology. 1987. V. 134. No. 12. Pp. 2953 - 2960. https://doi.org/10.1149/1.2100322

10.Yeliseyev V. I., Sovit Yu. Change in the potential of a liquid battery on external circuit closing. Bulletin of Dnipro University. Series: Mechanics. 2021. Iss. 25. Pp. 54 - 65. (in Ukrainian).

11. Yi Zeng. Mathematical Modeling of Lithium-Ion Intercalation Particles and Their Electrochemical Dynamics. Ph.D. Thesis. Massachusetts Institute of Technology, 2015. URL: https://dspace.mit.edu/handle/1721.1/99062 (Last accessed on April 28, 2023)

12. Yeliseyev V. I., Sovit Yu. P., Bliuss B. A. Ion transfer in convective/diffusion flow separation. In: Aerospace Hardware System Design and Performance Analysis. V. XXVI. Dnipro, 2019. Pp. 21-38. (in Ukrainian).

13. Shah A.A., Li X., Wills R.G.A., Walsh F.C. A mathematical model for the soluble lead-acid flow battery. J. of the Electrochemical Society. 2010. V. 157. No. 5. Pp. A589 - A599. https://doi.org/10.1149/1.3328520

14. Beneš M., Fučík R., Havlena V., Klement V., Kolář M., Polívka O., Solovský J, Strachota P. An efficient and robust numerical solution of the full-order multiscale model of lithium-ion battery. Mathematical Problems in Engineering. 2018. Article ID 3530975. https://doi.org/10.1155/2018/3530975

15. Apostolova R. D., Zadorei N. D., Kolomoets O. V., Shembel E. M. Comparative assessment of electrochemical sulfides' electrochemical conversion efficiency in a prototype lithium battery depending on the nature of the liquid electrolyte. Voprosy Khimii i Khimicheskoi Tekhnologii. 2012. No. 2. Pp. 186-190. (in Russian). URL: https://udhtu.edu.ua/public/userfiles/file/VHHT/2012/2/%D0%90postolova.pdf (Last accessed on April 28, 2023).

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