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Submitted on 30.01.14

Іванісік А., канд. фіз.-мат. наук, Ісаєнко О., асп., Коротков П., д-р фіз.-мат. наук, радіофізичний факультет, кафедра медичної радіофізики Київський національний університет імені Тараса Шевченка, Понежа Г., канд. фіз.-мат. наук, економіко-статистичний факультет, Національна академія статистики, обліку та аудиту

ФАЗОВА САМОМОДУЛЯЦІЯ ЛАЗЕРНОГО ІМПУЛЬСУ В ШАРУВАТИХ САМОФОКУСУЮЧИХ СЕРЕДОВИЩАХ

У роботі розглянуто фазову само модуляцію за квазістаціонарного самофокусування у шаруватій керрієвській рідині, розділеній оптично однорідним (нерозсіюючим) прошарком. Обраховано миттєву частоту імпульсу лазерного випромінювання в момент перетину області самофокусування тонкого прозорого шару. Додатково враховано поглинання світла на шарі.

Перехідне випромінювання на прошарку (скляній пластинці або подібній структурі), розміщеному в самофокусуєчому середовищі, має спільні характеристики з випромінюванням на виході із середовища. Зсув частоти перехідного випромінювання, що вишло із шару, менший за зсув частоти лазерного випромінювання на виході із середовища. Враховуючи, що прошарків може бути кілька, виявляється, що введення шарів у середовище спрощує експериментальне дослідження та застосування перехідного випромінювання.

Ключові слова: лазер, самофокусування, фазова само модуляція, перехідний ефект

Иванисик А., канд. физ.-мат. наук, Исаенко А., асп., Коротков П., д-р физ.-мат. наук, радиофизический факультет, кафедра медицинской радиофизики, Киевский национальный университет имени Тараса Шевченко, Понежа Г., канд. физ.-мат. наук, экономико-статистический факультет, Национальная академия статистики, учета и аудита

ФАЗОВАЯ САМОМОДУЛЯЦИЯ ЛАЗЕРНОГО ИМПУЛЬСА В СЛОИСТЫХ САМОФОКУСИРУЮЩИХ СРЕДАХ

В работе рассмотрена фазовая само модуляция в случае квазистационарной самофокусировки в слоистой керровской жидкости, разделенной оптически однородным (нерассеивающим) слоем. Рассчитана мгновенная частота импульса лазерного излучения в момент перехода области самофокусировки через тонкий прозрачный слой. Дополнительно учтено поглощение света на слое.

Переходное излучение на слое (стеклянной пластинке или подобной структуре), размещенном в самофокусирующей среде, имеет общие характеристики с излучением на выходе из среды. Смещение частоты переходного излучения, вышедшего из слоя, меньше сдвига частоты лазерного излучения на выходе из среды. Учитывая, что слоев может быть несколько, оказывается, что введение слоев в среду упрощает экспериментальное исследование и применение переходного излучения.

Ключевые слова: лазер, самофокусировка, фазовая само модуляция, переходный эффект

UDC 532,533, 533.9, 530.182

P. Kostrobij, Sc.D., B. Markovych, Ph.D., R. Tokarchuk, assist., Department of Applied Mathematics, Institute of Applied Mathematics and Fundamental Sciences, Lviv Polytechnic National University, Yu. Chernomorets, Ph.D. stud., Department of Nonequilibrium Processes Theory, Institute for Condensed Matter Physics, NAS of Ukraine M. Tokarchuk, Sc.D., Department of Applied Mathematics, Institute of Applied Mathematics and Fundamental Sciences, Lviv Polytechnic National University, Department of Nonequilibrium Processes Theory, Institute for Condensed Matter Physics, NAS of Ukraine

STATISTICAL THEORY OF ELECTRO-DIFFUSION PROCESSES OF IONS INTERCALATION IN "ELECTROLYTE – ELECTRODE" SYSTEM

A statistical theory of classical-quantum description of electro-diffusion processes of intercalation in "electrolyte-electrode" system is proposed. Using the nonequilibrium statistical operator method the generalized transport equations of Nernst-Planck type for ions and electrons in the "electrolyte-electrode" system are obtained. These equations take into account time memory effects and spatial heterogeneity. A one-dimensional simplified model of intercalation of ions into the electrode structure with taking the dielectric polarization into account is proposed.

Keywords: electrolyte, electrode, intercalation, nonequilibrium statistical operator .

1. Introduction. Theoretical studies of electro-diffusion transport processes of ions and electrons in the "electrode-electrolyte" systems remain actual nowadays [6, 16, 19]. They are linked with a need to describe nonequilibrium processes of intercalation as well as to develop a theory suitable for practical application to predicting and controlling these processes. The difficulties in describing processes at electrode are first of all related with surface phenomena at electrolyte-electrode interface. In this region, complicated processes of adsorption and diffusion take place which are connected with a problem of charge accumulation at battery electrodes. In the system "electrode (anode)-electrolyte-electrode (cathode)", the anode plays role of the source of both electrons, which move to cathode by the corresponding electric circle, and lithium ions in electrolyte. A cathode is typically a metallic

system (nickel, for example) covered with active material containing carbon and in which lithium ions intercalate from the solution. Herewith, an important issue is the following one. The electrochemical processes in electrolyte solution can be described using methods of classical statistical mechanics, whereas in the region near the electrolyte-electrode interface and inside the electrodes, description of diffusion and intercalation processes should be implemented by means of the modern methods of quantum statistical physics. In this field, the electrochemical impedance studies [4, 1, 8] of electro-diffusion transport processes in Li-ion batteries [18, 9, 10] were carried out and intercalation/deintercalation processes were investigated using nonequilibrium thermodynamics [19, 9, 2, 17]. The theoretical and experimental studies of chemical diffusion coefficient for lithium ions in intercalation

processes into various electrode materials are actively carried out [12, 20, 5, 7, 15]. A complicated dependence of chemical diffusion coefficient on a degree of electrochemical intercalation and on alteration of structure of cathode material is analyzed as well. In particular, in Ref. [12] based on a detailed analysis of experimental investigations for various materials an important conclusion was drawn: the structure of intercalated material has the main influence on the chemical diffusion coefficient. Consequently, it is important to take into account to some extent the altering of microstructure of cathode material, in particular, via its polarization properties.

2. Generalized transport Nernst-Planck equations

$$\frac{\partial}{\partial t} \delta n_{\alpha}(\vec{r}_i; t) = \frac{\partial}{\partial \vec{r}_i} \cdot (\vec{j}_{\alpha}^{(1)}(\vec{r}_i; t) + \vec{j}_{\alpha}^{(2)}(\vec{r}_i; t) + \vec{j}_{\alpha}^{(3)}(\vec{r}_i; t)),$$

where the ion flows have the following structure [19]:

$$\begin{aligned} \vec{j}_{\alpha}^{(1)}(\vec{r}_i; t) &= \sum_{l' \gamma} \int d\vec{r}_{l'} \int_{-\infty}^t e^{\varepsilon(t'-t)} \beta D_{jj}^{\alpha \gamma}(\vec{r}_i, \vec{r}_{l'}; t, t') \times \frac{\partial}{\partial \vec{r}_{l'}} Z_{\gamma} e \phi(\vec{r}_i; t') dt' - \int d\vec{r}_{s'} \int_{-\infty}^t e^{\varepsilon(t'-t)} \beta D_{jj}^{\alpha e}(\vec{r}_i, \vec{r}_{s'}; t, t') \cdot \frac{\partial}{\partial \vec{r}_{s'}} e \phi(\vec{r}_{s'}; t') dt' \\ \vec{j}_{\alpha}^{(2)}(\vec{r}_i; t) &= \sum_{l' \gamma} \int d\vec{r}_{l'} \sum_{l'' \alpha'} \int d\vec{r}_{l''} \int_{-\infty}^t e^{\varepsilon(t'-t)} \beta D_{jj}^{\alpha \alpha'}(\vec{r}_i, \vec{r}_{l''}; t, t') \times \frac{\partial}{\partial \vec{r}_{l''}} [\tilde{\Phi}_d^{-1}(\vec{r}_i, \vec{r}_{l''}; t')]_{\alpha, \gamma} \delta n_{\gamma}(\vec{r}_{l''}; t') dt' \\ &\quad - \int d\vec{r}_{s'} \int d\vec{r}_{s''} \int_{-\infty}^t e^{\varepsilon(t'-t)} \beta D_{jj}^{\alpha e}(\vec{r}_i, \vec{r}_{s''}; t, t') \times \frac{\partial}{\partial \vec{r}_{s''}} [\tilde{\Phi}_d^{-1}(\vec{r}_i, \vec{r}_{s''}; t')]_{ee} \delta \bar{n}_e(\vec{r}_{s''}; t') dt' \\ \vec{j}_{\alpha}^{(3)}(\vec{r}_i; t) &= \sum_{l' \gamma} \int d\vec{r}_{l'} \sum_{l'' \alpha'} \int d\vec{r}_{l''} \int_{-\infty}^t e^{\varepsilon(t'-t)} \beta \times \bar{D}_{jjn}^{\alpha \alpha' \gamma}(\vec{r}_i, \vec{r}_{l''}; t, t') \cdot \frac{\partial}{\partial \vec{r}_{l''}} Z_{\alpha'} e \phi(\vec{r}_{l''}; t') \delta n_{\gamma}(\vec{r}_{l''}; t') dt' + \sum_{l' \gamma} \int d\vec{r}_{l'} \int d\vec{r}_{s'} \int_{-\infty}^t e^{\varepsilon(t'-t)} \beta \bar{D}_{jjn}^{\alpha e}(\vec{r}_i, \vec{r}_{l'}, \vec{r}_{s'}; t, t') \\ &\quad \times \frac{\partial}{\partial \vec{r}_{l'}} Z_{\gamma} e \phi(\vec{r}_{l'}; t') \delta \bar{n}_e(\vec{r}_{s'}; t') dt' - \sum_{l' \gamma} \int d\vec{r}_{l'} \int d\vec{r}_{s'} \int_{-\infty}^t e^{\varepsilon(t'-t)} \beta \bar{D}_{jjn}^{\alpha \gamma}(\vec{r}_i, \vec{r}_{s'}; t, t') \\ &\quad \times \frac{\partial}{\partial \vec{r}_{s'}} e \phi(\vec{r}_{s'}; t') \delta n_{\gamma}(\vec{r}_{l'}; t') dt' - \int d\vec{r}_{s'} \int d\vec{r}_{s''} \int_{-\infty}^t e^{\varepsilon(t'-t)} \beta \bar{D}_{jjn}^{\alpha ee}(\vec{r}_i, \vec{r}_{s''}; t, t') \times \frac{\partial}{\partial \vec{r}_{s''}} e \phi(\vec{r}_{s''}; t') \delta \bar{n}_e(\vec{r}_{s'}; t') dt' \end{aligned}$$

Here z_{γ} is ion of valence and e is the electron charge; $\phi(\vec{r}_i; t')$ and $\phi(\vec{r}_{s'}; t')$ are scalar potentials of the electromagnetic field, which during the charging/discharging of batteries are the driving forces of transport processes of ions in the electrolyte and intercalated ions and electrons in the electrode.

These equations take into account the time memory effects and spatial heterogeneity. An important contribution to the generalized Nernst-Planck type equations are provided by the transport kernels which, unlike the generalized diffusion coefficients, are the third-order correlation functions and enter into equations via terms of second order in the parameters which describe the dynamic correlations between the field and a density.

$$D_{jj}^{\alpha \gamma}(\vec{r}_i, \vec{r}_{l'}; t, t') = \langle (1 - P(t)) \hat{j}_{\alpha}(\vec{r}_i) T_q(t, t') (1 - P(t')) \hat{j}_{\gamma}(\vec{r}_{l'}) \rangle_{q'}^t$$

is the generalized diffusion coefficient of ions as a function of coordinates and time. When $l = f$ and $l' = f'$, we have diffusion coefficient in electrolyte solution.

$$\hat{j}_{\alpha}(\vec{r}_i) = \frac{1}{m_{\alpha}} \sum_{j=1}^{N_{\alpha}} \vec{p}_j \delta(\vec{r}_i - \vec{r}_j)$$

is the current density of ions of species α in the electrolyte solution. When $l = s$ and $l' = s'$, we have a cross-diffusion coefficient for ions in the electrolyte solution and electrode. In this case,

$$\hat{j}_{\alpha}(\vec{r}_s) = \frac{1}{m_{\alpha}} (\hat{\psi}_{\alpha}^{+}(\vec{r}_s) \nabla_s \hat{\psi}_{\alpha}(\vec{r}_s) - \nabla_s \hat{\psi}_{\alpha}^{+}(\vec{r}_s) \hat{\psi}_{\alpha}(\vec{r}_s))$$

is the operator of current density of ions in the electrode

We proposed a statistical theory of classical-quantum description of electro-diffusion transport processes of ions and electrons in the "electrolyte-electrode" system [13] using the D. Zubarev nonequilibrium statistical operator (NSO) method [14, 21]. The presented theory takes the spatial heterogeneity and memory effects into account. The model and corresponding Hamiltonian are formulated and the nonequilibrium statistical operator for the "electrolyte-electrode" system as the functional of the corresponding parameters of the reduced description of the nonequilibrium processes (observable parameters) is obtained. In this approach, we receive the generalized transport equations such as Nernst-Planck equation for electrons and ions in the "electrolyte-electrode" system using the method of nonequilibrium statistical operator:

structure. When $l = s$ and $l' = s'$, we have the generalized quantum diffusion coefficient for ions in the electrode subsystem:

$$\begin{aligned} D_{jj}^{\alpha e}(\vec{r}_i, \vec{r}_{s'}; t, t') &= \langle (1 - P(t)) \hat{j}_{\alpha}(\vec{r}_i) T_q(t, t') \\ &\quad \times \int_0^1 d\tau \rho_{\phi}^{-1}(\tau) (1 - P(t')) \hat{j}_{e}(\vec{r}_{s'}) \rho_{\phi}^{-1}(\tau) \rangle_{\phi}^t \end{aligned}$$

defines a generalized of ion-electron diffusion, herewith, ion can be in the electrolyte subsystem or in the electrode one. $\rho_{\phi}(\tau)$ is the quasiequilibrium statistical operator. In the generalized Nernst-Planck equations an important role belongs to transport kernels

$$\begin{aligned} D_{jjn}^{\alpha \alpha' \gamma}(\vec{r}_i, \vec{r}_{l'}, \vec{r}_{l''}; t, t') &= \sum_{l'' \alpha''} \int d\vec{r}_{l''} \langle (1 - P(t)) \hat{j}_{\alpha}(\vec{r}_i) T_q(t, t') \\ &\quad \times (1 - P(t')) \hat{j}_{\alpha'}(\vec{r}_{l''}) \hat{n}_{\alpha''}(\vec{r}_{l''}) \rangle_{\phi}^t [\tilde{\Phi}_d^{-1}(\vec{r}_i, \vec{r}_{l''}; t')]_{\alpha, \gamma} \end{aligned}$$

Unlike the transport kernels related with the generalized coefficient, they are the correlation functions of the third order and enter into the equations via the second order in the parameters $\phi(\vec{r}_i; t') \delta n_{\gamma}(\vec{r}_{l''}; t')$, $\phi(\vec{r}_i; t') \delta \bar{n}_e(\vec{r}_{s'}; t')$, $\phi(\vec{r}_{s'}; t') \delta \bar{n}_e(\vec{r}_{s''}; t')$. We also obtained the system of equations for the flows of ions and electrons from which the conditions of the existence of stationary processes can be determined. Approximate calculation of diffusion coefficients by means of the method of moments in Gaussian approximation provides us the relationship between the unary and pair distribution functions of quasiequilibrium state.

3. One-dimensional model of intercalation of ions into the electrode structure with taking the dielectric polarization into account In the generalized Nernst-Planck equations that describe the transport processes of ions and electrons in the "electrolyte-electrode" system with spatial heterogeneity and memory effects in time polarization processes are taken into account [13] by the averaged Maxwell's equations for the electromagnetic field. Based on this approach, we consider a simplified model of ion intercalation based on the Nernst-Planck equation, excluding electronic component and memory effects in time. That is, we consider a one-dimensional model with diagram shown in Figure

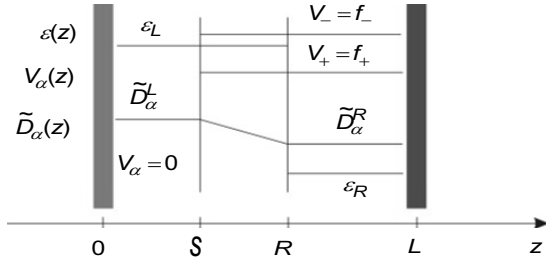


Fig. 1. Diagram of the "electrode-electrolyte" systems

We describe transport processes of ions between the electrodes by the Nernst-Planck equations

$$\frac{\partial}{\partial t} n_{\alpha}(z;t) = \frac{\partial}{\partial z} [\tilde{D}_{\alpha}(z;t) [\frac{\partial}{\partial z} n_{\alpha}(z;t) + n_{\alpha}(z;t) (\frac{\partial}{\partial z} V_{\alpha}(z) + Z_{\alpha} e \frac{\partial}{\partial z} \phi(z;t))]]$$

where $\tilde{D}_{\alpha}(z;t)$ is the mobility of ions of class α , $V_{\alpha}(z)$ is the surface potential of two phases electrolyte-electrode, $\phi(z;t)$ is the electric potential which satisfies the Poisson equation

$$-\frac{\partial}{\partial z} (\epsilon(z) \frac{\partial}{\partial z} \phi(z;t)) = 4\pi \sum_{\alpha} Z_{\alpha} e n_{\alpha}(z;t)$$

under the conditions $\bar{j}_{\alpha}(0;t) = \bar{j}_{\alpha}(L;t)$, $\phi(0) = \phi_0$, $\phi(L) = \phi_L$. The time dependence of the potentials on electrodes we present in the form

$$\phi_0(t) = -\phi_L(t) = \phi^{st} + \frac{1}{2} (\phi e^{i\omega t} + c.c.),$$

where ϕ^{st} is a static potential, and $\phi_0(\omega) = \frac{\phi}{2}$. Then the voltage between the electrodes is equal to

$$U(t) = \phi_0(t) - \phi_L(t) = 2\phi^{st} + U(\omega) e^{i\omega t} + c.c.$$

$U(\omega) = \phi$. Using Gauss's law for vector of the electric displacement $D(z;t)$ at $z=0$ we find the density of the surface charge:

$$\sigma_0(t) = -\frac{\epsilon(0)}{4\pi} \frac{\partial}{\partial z} \phi(z;t)|_{z=0} = D(0;t) = \sigma_0^{st} + \frac{1}{2} (\sigma_0^{am} e^{i\omega t} + c.c.),$$

σ_0^{am} is the peak value. Next we narrow the model of two-component ionic solution $Z_{\alpha} = Z_{+}, Z_{-}$ with the interfacial area $z = R$, $z = S$ and with the corresponding values of the dielectric function and surface potential:

$$\epsilon(z) = \begin{cases} \epsilon_L, & z < R \\ \epsilon_R, & z > R \end{cases}$$

$$V_{\pm}(z) = \begin{cases} 0, & z < S \\ f_{\pm}, & z > S \end{cases}$$

where $|R-S| \ll L$, and f_{\pm} is the ions solubility in the corresponding phase. The mobility of ions is specified in each phase:

$$\tilde{D}_{\pm} = \begin{cases} \tilde{D}_{\pm}^L, & z < \min(R, S) \\ \tilde{D}_{\pm}^R, & z > \max(R, S) \end{cases}$$

First we consider the case of constant voltage over time:

$$\phi_0(t) = -\phi_L(t) = \phi^{st},$$

with the condition $j_{\pm}(0;t) = j_{\pm}(L;t)$. In the homogeneous case a Poisson equation has the form:

$$-\frac{\partial}{\partial z} (\epsilon(z) \frac{\partial}{\partial z} \phi_{\text{hom}}(z;t)) = 0.$$

Its analytical solution can be represented as:

$$\phi_{\text{hom}}(z) = \begin{cases} \frac{A_L}{\epsilon_L} z + B_L, & z < R \\ \frac{A_R}{\epsilon_R} z + B_R, & z > R \end{cases}$$

with the conditions of the continuity

$$\begin{aligned} D(R^{-};t) &= D(R^{+};t) = \epsilon_L \frac{\partial}{\partial z} \phi(z;t)|_{z=R^{-}} \\ &= \epsilon_L \frac{\partial}{\partial z} \phi(z;t)|_{z=R^{+}} \end{aligned}$$

$\phi(R^{-};t) = \phi(R^{+};t)$. As a result, the solution will look like:

$$\phi_{\text{hom}}(z;t) = \begin{cases} -\frac{2\phi^{st}}{\epsilon_L} \left(\frac{R}{\epsilon_L} + \frac{L-R}{\epsilon_R}\right)^{-1} z + \phi^{st}, & z < R \\ \frac{2\phi^{st}}{\epsilon_R} \left(\frac{R}{\epsilon_L} + \frac{L-R}{\epsilon_R}\right)^{-1} (L-z) - \phi^{st}, & z > R \end{cases}$$

Then we find the solution of the inhomogeneous Poisson equation using the Green's functions method:

$$\frac{\partial}{\partial z} (\epsilon(z) \frac{\partial}{\partial z} G(z, z')) = -4\pi \delta(z - z')$$

with the boundary conditions

$$G(0, z') = 0 \quad G(R^{-}, z') = G(R^{+}, z')$$

$$G(L, z') = 0 \quad \epsilon_L \frac{\partial}{\partial z} G(z = R^{-}, z') = \epsilon_R \frac{\partial}{\partial z} G(z = R^{+}, z').$$

The result is:

$$G(z, z') = \begin{cases} -\frac{4\pi}{\epsilon_L} \Theta(z - z') (z - z') - \frac{C(z')}{\epsilon_L} z, & z < R \\ -\frac{4\pi}{\epsilon_R} \Theta(z - z') (z - z') - \frac{C(z')}{\epsilon_R} z, & z > R \\ +\frac{4\pi}{\epsilon_R} (L - z') + \frac{L}{\epsilon_R} C(z'), & z > R \end{cases}$$

where

$$C(z') = \frac{4\pi}{\epsilon_R - \epsilon_L} [\Theta(R - z') (R - z') \left(\frac{1}{\epsilon_L} - \frac{1}{\epsilon_R}\right) + (L - z') \frac{1}{\epsilon_R}]$$

Then the solution of Poisson's equation for the selected model can be represented as:

$$\phi(z;t) = \phi_{\text{hom}}(z;t) + \int_0^L dz' G(z, z') (n_{+}(z';t) - n_{-}(z';t)).$$

Thus, substituting present solution to the Nernst-Planck equation, we get a closed system of equations:

$$\begin{aligned} \frac{\partial}{\partial t} n_{\alpha}(z;t) &= \frac{\partial}{\partial z} [\Omega_{\alpha}(z;t) \left[\frac{\partial}{\partial z} n_{\alpha}(z;t) + \right. \\ n_{\alpha}(z;t) \left(\frac{\partial}{\partial z} V_{\alpha}(z) + Z_{\alpha} e \frac{\partial}{\partial z} (\phi_{\text{hom}}(z;t) + \right. & \quad (1) \\ \left. \left. \int_0^L dz' G(z,z') (n_{+}(z';t) - n_{-}(z';t)) \right) \right] \end{aligned}$$

under the certain mobilities of ions $\bar{D}_{\alpha}(z;t)$ and the surface potential $V_{\alpha}(z)$. The system of equations is nonlinear. An important step is to study the solutions of the system of equations close to equilibrium when $n_{\alpha}(z;t) = n_{\alpha}^{\text{st}}(z)$ is static distribution of ions in the "electrolyte-electrode" system. Solutions of the system of equations (1) for the approximate calculation $\bar{D}_{\alpha}(z;t) \approx \frac{\beta}{m_{\alpha}} n_{\alpha}(z;t)$ through the moments [13] may be important that requires some mathematical research.

4. Conclusions. Summarizing, we proposed a statistical theory of classical-quantum description of electrodiffusion transport processes of ions and electrons in the "electrolyte- electrode" system using the NSO method. The presented theory takes the spatial heterogeneity and memory effects into account. In this approach, we receive the generalized transport equations such as Nernst-Planck equation for electrons and ions in the "electrolyte-electrode" system using the method of nonequilibrium statistical operator. These equations take into account the time memory effects and spatial heterogeneity. An important contributions to the generalized Nernst-Planck type equations are provided by the transport kernels $\bar{D}_{jn}^{\alpha\alpha' \gamma}$, which, unlike the generalized diffusion coefficients, are the third-order correlation functions and enter into equations via terms of second order in the parameters $\varphi(\vec{r}_i;t) \delta n_{\gamma}(\vec{r}_i;t)$, $\varphi(\vec{r}_i;t) \delta \bar{n}_{\alpha}(\vec{r}_s;t)$, $\varphi(\vec{r}_s;t) \delta \bar{n}_{\alpha}(\vec{r}_s;t)$ which describe the dynamic correlations between the field and a density.

In this approach, we have considered a one-dimensional simplified model of intercalation of ions into the electrode structure with taking the dielectric polarization into account.

An important open issue consists in the appearance of bound states of Li ions with electrons and Li ions inside electrode. For description of such processes, the transport equations should be complemented with the equations for "ion-ion", "ion-electron" and "electron-electron" nonequilibrium pair distribution functions within the electrode structure. These problems we will consider in our future works. Besides, within the classical description of an electrolyte we did not consider explicitly polar molecules of solvent which, evidently, can significantly effect the polarization processes due to their orientational movement and can be transported into the porous structure of electrode (what leads to a decrease of porosity and cleavage). This needs a separate study as well.

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Submitted on 04.11.14

Костробий П., д-р фіз.-мат. наук, Маркович Б., канд. фіз.-мат. наук
Токарчук Р., асист., каф. прикладної математики,
Інститут прикладної математики та фундаментальних наук, Національний університет "Львівська політехніка",
Черноморець Ю., асп., відділ теорії нерівноважних процесів, Інститут фізики конденсованих систем НАН України,
Токарчук М., д-р фіз.-мат. наук, каф. прикладної математики,
Інститут прикладної математики та фундаментальних наук, Національний університет "Львівська політехніка",
відділ теорії нерівноважних процесів, Інститут фізики конденсованих систем НАН України

СТАТИСТИЧНА ТЕОРІЯ ЕЛЕКТРОДИFUЗІЙНИХ ПРОЦЕСІВ ІНТЕРКАЛЯЦІЇ ІОНІВ В СИСТЕМІ "ЕЛЕКТРОЛІТ-ЕЛЕКТРОД"

Запропоновано статистичну теорію для класично-квантового опису електроди фузійних процесів інтеркаляції в системі "електроліт-електрод". Використовуючи метод нерівноважного статистичного оператора, отримано узагальнені рівняння переносу типу Нернста-Планка для іонів та електронів в системі "електроліт-електрод". Ці рівняння враховують ефекти пам'яті в часі та просторову неоднорідність. Запропоновано одомірну спрощену модель інтеркаляції іонів в структуру електрода з врахуванням діелектричної поляризації.

Ключові слова: електроліт, електрод, інтеркаляція, нерівноважний статистичний оператор.

Костробий П., д-р фіз.-мат. наук, Маркович Б., канд. фіз.-мат. наук,
Токарчук Р., асист., каф. прикладної математики,
Інститут прикладної математики та фундаментальних наук, Національний університет "Львівська політехніка",
Черноморець Ю., асп., відділ теорії нерівноважних процесів, Інститут фізики конденсованих систем НАН України,
Токарчук М., д-р фіз.-мат. наук, каф. прикладної математики, Інститут прикладної математики та фундаментальних наук
Національний університет "Львівська політехніка", відділ теорії нерівноважних процесів,
Інститут фізики конденсованих систем НАН України

СТАТИСТИЧЕСКАЯ ТЕОРИЯ ЭЛЕКТРОДИFUЗИОННЫХ ПРОЦЕССОВ ИНТЕРКАЛЯЦИИ ИОНОВ В СИСТЕМЕ "ЭЛЕКТРОЛИТ-ЭЛЕКТРОД".

Предложено статистическую теорию для классическо-квантового описания электродиффузионных процессов интеркаляции в системе "электролит-электрод". Используя метод неравновесного статистического оператора, получены обобщенные уравнения переноса типа Нернста-Планка для ионов и электронов в системе "электролит-электрод". Эти уравнения учитывают эффекты памяти во времени и пространственную неоднородность. Предложено одомірную упрощенную модель интеркаляции ионов в структуру электродов с учетом диелектрической поляризации.

Ключевые слова: электролит, електрод, интеркаляція, неравновесный статистический оператор.