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The model of potential barrier appearing in a hydrolayer localized in a two-layer porous nanostructure

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Abstract. A model has been proposed to describe the potential barrier that appears during interaction of two compacted layers consisting of hydrophilic oxide nanoparticles of different sizes in each layer upon saturation of this structure with adsorbed water. The dependence of the space charge density of the compacted powder material on the density of particles in it has been theoretically calculated. The distribution of the potential over the thickness of contact between two layers consisting of nanoparticles with different sizes has been obtained.

Keywords: potential barrier, two-layer porous structure, hydrated layer, nanoparticles.

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1. Introduction

Currently, there is a growing need to search for new materials and structures based on these materials to optimize the flow of energy conversion processes in fuel and electrochemical cells, as well as in new energy sources that will be used in branches of industry where it is impractical to use traditional sources consuming energy from fossil natural resources. One of the possible solutions to this problem can be the use of modern powder nanotechnology, in particular, compacted nanodispersed hydrophilic materials.

In a number of works [1–3], the appearance of free charge carriers on the surface of a nanodispersed metal oxide (MeO_2) powder during adsorption of water was considered. In this case, the material MeO_2 itself is dielectric with a large bandgap value. However, when an electrically neutral nanoparticle of a hydrophilic metal oxide is deposited onto the surface, a neutral water molecule under the action of intermolecular forces (van der Waals forces) dissociates into protons H^+ and OH^- groups. This means that the following electrochemical process is realized:

$$H_2O + e^- \rightarrow H^+ + OH^-. \quad (1)$$

When atoms or molecules are adsorbed on the ideal surface of a solid, local electronic states appear. An adsorbed particle can either capture electron, acting as a surface acceptor, or give electron to the crystal as a donor. As a result, a double electric layer of adsorption origin (Helmholtz layer) is formed around the particle, and the surface of the nanoparticles acquires a negative charge. On the contrary, the outer more rarefied diffuse layer carries a potential that arises in it due to redistribution of ions of opposite charge.

Based on this effect, several models of the structure of compressed nanodispersed MeO_2 powder were proposed, the potential difference on the surface of which is caused by the moisture gradient in it [4–6], *i.e.*, the structure acts as an analogue of an electrochemical capacitor. However, after complete saturation of the structure with moisture or its drying, the potential difference on opposite surfaces of the structure disappears, which is due to the practically identical or very close density of surface states of particles, the geometric dimensions of which fall into a very narrow range of values.

In this regard, behavior of a structure consisting of several layers of compressed nanodispersed powder, each layer of which consists of particles with different sizes and, as a consequence, with a different surface area of particles in each layer, is of interest. If the surface area of the particles in different layers is very different, and the density of surface states is the same, since the material is the same in both layers, then the resulting structure should exhibit the properties of a heterostructure. In this case, the potential difference on opposite surfaces of the heterostructure will be caused not only by the moisture gradient in it, but also by the different number of adsorbed water molecules in each layer.

In this work, we consider a model of a potential barrier in a heterostructure consisting of two layers of compressed nanodispersed hydrophilic powder (similar to nanodispersed metal oxides) with different particle sizes in each layer on saturation of this structure with water. After saturation with moisture, the water around the particles will begin to form a double layer, and it can be assumed that the surface of the particles will be negatively charged with a certain surface density. The space between the particles will be filled with positive H^+ ions. The specific surface area and the density of the surface charge on particles of various sizes are different, therefore, in general, for the layers consisting of particles with different sizes, different charges and concentration of protons can be observed.

Separately, these layers will be electrically neutral, but after being brought into contact, in a small area near the interface, a concentration gradient of positive charges arises, causing them to move from places with a higher concentration to a zone with a lower one. The appearance of additional ions in the area with a lower concentration violates the balance of charges on the particle surface and in the interparticle space, and, therefore, an excess of positive charge arises. Similarly, in another layer of particles, an imbalance is observed with respect to appearance of a total negative charge equal in its magnitude.

2. Mathematical model

A cylindrical tablet with the height h_V = 1 mm and diameter d_V = 1 cm, consisting of two layers of pressed ultrafine-grained powders with an average particle size of 10 nm and 20 nm in diameter, is considered as a model of a two-layer structure for computer simulation.

The specific surface of the particles is different, and therefore the surface charge on the particles will be different. In addition, due to the different sizes, different numbers of particles will fall into the limited space of the extruded structure and, therefore, the total charge of the layers will differ. In the entire space of the structure, the negative charge on the particle surface will be practically compensated by the positive charge of the double layer, but in the area of direct contact of the layers, diffusion of positive radicals will occur, due to which the concentration of negative and positive charges will be redistributed in this area.

To estimate the distribution of the electrostatic potential φ arising inside the space charge region (SCR), it is necessary to solve the Poisson equation inside two charged cylinders in contact with each other:

$$\int \Delta\varphi dV = -\left(\frac{\int \rho_{macro10}}{\varepsilon_{10}\varepsilon_0} dV_{10} + \frac{\int \rho_{macro20}}{\varepsilon_{20}\varepsilon_0} dV_{20} \right), \qquad (2)$$

where $\rho_{macro10,20}$ is the space charge density in the corresponding layer of particles in powder, $\varepsilon_{10,20}$ – dielectric permittivity inside the layers, $V_{10,20}$, V are the volumes of the layers and the total volume of the investigated area, respectively, ε_0 is the dielectric permittivity of SI.

The potential distribution can be considered in more detail when modeling specific layers of particles with a negative charge on the particle surface and a positive charge in the interparticle space or when solving the equation for a more general case:

$$\int \Delta\varphi dV = -\left(\begin{array}{l} \dfrac{\int \rho_{macro10}}{\varepsilon_{10}\varepsilon_0} dV_{10} + \dfrac{\int \rho_{macro20}}{\varepsilon_{20}\varepsilon_0} dV_{20} + \\ + \sum^{N_{10}} \int \sigma_{10} dS_{10} + \sum^{N_{20}} \int \sigma_{20} dS_{20} \end{array} \right), \qquad (3)$$

where $\rho_{micro10.20}$ is the space charge density of the interparticle space of the powder, $\sigma_{10.20}$ – surface charge density, $S_{10.20}$ – surface of particles with the corresponding size, $N_{10.20}$ – number of particles in the layer.

Since the structure under study is a system of particles with the same surface charge density, the total charge in the same volume will depend on the number of particles contained in each layer separately:

$$q = 4\pi \cdot R^2 \cdot \sigma \cdot N\ , \qquad (4)$$

where σ is the surface charge of a nanoparticle, R – radius of the particle, and N – number of particles in a fixed volume.

When the powder is compacted, the particles in the layer will be arranged according to the principle of close packing. Suppose that in a separate layer all particles are spherical and are at the same distance from each other. This is a known problem of close packing of identical spheres. It is argued that in a closed space the same spheres can occupy a position in the form of a face-centered cubic (FCC) lattice and a hexagonal close-packed (HCP) lattice, and this position will be the most dense [7]. Both packings are similar in orientation in the same plane – the distance between the centers of neighboring spheres is the same – but HCP is a usual combination of two layers (instead of three layers in FCC), which is repeated and differs only by a spatial shift by the value of the radius.

Obviously, for transition from FCC packing to HCP packing, only one layer needs to be moved back. Therefore, they do not differ in the maximum packing density, and this value equals:

$$D_{\max} = \frac{\pi}{3\sqrt{2}} \approx 0.74\,. \qquad (5)$$

The hypothesis that these packets have the highest density among all possible regular and irregular packets of spheres in three-dimensional space was confirmed in 2005 [8].

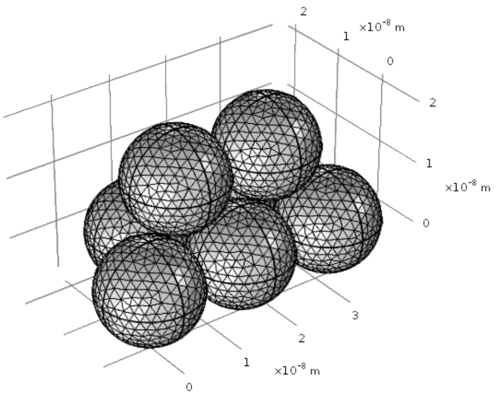

Fig. 1. Model of compaction of particles.

To estimate the number of spherical particles in a cylinder of known volume, we assume that they occupy a position similar to HCP, so that their centers can be represented by the nodes of a regular tetrahedron with a side length of $2R + d$, where d is the distance between the particle boundaries. In this case, at the distance $d = 0$, the particles occupy the position shown in Fig. 1.

Thus, we can estimate the integer number of particles falling into a certain volume V

$$n_z = \frac{h_V}{k(2R+d)} - \frac{1-k}{k},$$

$$n_{x,y} = \frac{d_V}{k(2R+d)}, \qquad (6)$$

where n_z is the number of particles along the height of the volume h_V, $n_{x,y}$ – number of particles along the d_V line in the plane, k – compaction coefficient, responsible for how far the layers of particles are above each other. In the case of compaction of particles in the form of an HCP lattice, this distance is the height of the tetrahedron, therefore, $k = \sqrt{\frac{2}{3}}$ $k \in \begin{Bmatrix} \sqrt{3} \\ 2.1 \end{Bmatrix}$ is the coefficient of compaction of particles in the plane.

Due to the fact that the particle size is rather small as compared to the characteristic size of the area under consideration, the number of particles N can be determined by the formula for the volume of a cylinder/parallelepiped:

$$N = C \cdot n_x \cdot n_y \cdot n_z = C \frac{d_V^2}{\frac{\sqrt{3}}{2}(2R+d)^2} \left(\frac{h_V}{k(2R+d)} - \frac{1-k}{k} \right),$$

$$C \in \begin{Bmatrix} \pi \\ 4.1 \end{Bmatrix} \qquad (7)$$

for n_x and n_y the values of k are different: $k = 1$ for n_x, $k = \frac{\sqrt{3}}{2}$ for n_y, C – parameter reflecting the geometry of the structure (cylinder or parallelepiped). The volume of the particle $V_{particle}$ and the volume of the selected area of the layer V of nanoparticles can be calculated by the formulas:

$$V_{particle} = \frac{4}{3} \pi \cdot R^3 \cdot N, \; V = h \cdot d_{bulk}^2 \cdot C. \qquad (8)$$

Since a system of particles located at a certain distance from each other can be considered as porous, it is necessary to determine the dielectric permittivity depending on the porosity of the material P [9]:

$$\varepsilon_{por} = \frac{2 \cdot (1-P) \cdot (\varepsilon_{particle} - 1) + \varepsilon_{particle} + 2}{\varepsilon_{particle} + 2 - (1-P) \cdot (\varepsilon_{particle} - 1)}, \qquad (9)$$

where $\varepsilon_{particle}$ is the dielectric permittivity of the nanoparticle, P – porosity of the particle layer.

The porosity of particle layer depends on the distance between particles.

$$P = 1 - \frac{V_{particle}}{V} =$$
$$= 1 - \frac{8\sqrt{3}\pi}{9} \cdot \frac{R^3}{h_V \cdot (2R+d)^2} \left(\frac{h_V}{k(2R+d)} - \frac{1-k}{k} \right). \qquad (10)$$

As can be seen, if the distance between the particles becomes $d = 0$, then the compaction density $D = 1 - P$ for particles with the sizes 10 and 20 nm is very close to the theoretical maximum (see the expression (5)), D_{10} ($R = 5$ nm) ≈ 0.726, D_{20} ($R = 10$ nm) ≈ 0.734.

By using the formula (4), it is possible to determine only the negative charge arising on the surface of the particles in the layer. In this case, in the contact area of layers of nanoparticles with different sizes, a part of positive charges flows from the layer with a higher charge into the layer with the lower one. Since the number of particles and specific surface in a layer of particles with the size 10 nm is larger, the charge at the interface of contact between the layers can be determined as

$$Q = \pm \frac{q_{10} - q_{20}}{2}. \qquad (11)$$

Then, with account of the formulas (4), (8), (10), the space charge density can be determined using the formula

$$\rho_{macro10,20} = \pm \frac{Q}{V_{10,20}} = \frac{2\pi}{C} \frac{R_{10}^2 \cdot \sigma_{10} \cdot N_{10} - R_{20} \cdot \sigma_{20} \cdot N_{20}}{h_{10,20} \cdot d_V^2} =$$
$$= \frac{3}{2h_{10,20}} \left((1-P_{10}) \cdot \sigma_{10} \cdot \frac{h_{10}}{R_{10}} - (1-P_{20}) \cdot \sigma_{20} \cdot \frac{H - h_{10}}{R_{20}} \right). \qquad (12)$$

Determination of the dimensions of the space charge region H is not the subject of this study. Further numerical calculations were carried out in the approximation that $H = h_{10} + h_{20} = 500$ nm, and the charge distributed over layers of nanoparticles with the thickness h_{10} and h_{20} equals $Q \approx 6 \cdot 10^{-10}$ C.

Using the formulas (4), (7), (11), one can obtain an expression for determining the thickness of the layer of powder particles, in which the charge Q is concentrated:

$$h_{10}=\frac{\dfrac{2\cdot Q\cdot\kappa\cdot k}{(\pi\cdot d_{bulk})^2}+\dfrac{R_{20}^2\cdot H\cdot\sigma_{20}}{(2\cdot R_{20}+d_{20})^3}+(1-k)\cdot\left(\dfrac{R_{10}^2\cdot\sigma_{10}}{(2\cdot R_{10}+d_{10})^2}-\dfrac{R_{20}^2\cdot\sigma_{20}}{(2\cdot R_{20}+d_{20})^2}\right)}{\dfrac{R_{10}^2\cdot\sigma_{10}}{(2\cdot R_{10}+d_{10})^3}+\dfrac{R_{20}^2\cdot\sigma_{20}}{(2\cdot R_{20}+d_{20})^3}}, \quad (13)$$

After we have determined the thickness of SCR, we can estimate the number of particles captured in the selected volume and developed a detailed model that recreates the structure described above.

3. Numerical simulation

A trial version of the COMSOL Multiphysics software package was used to solve this problem. For numerical calculations, the following parameters of the macromodel were chosen: the structure consists of two layers of nanoparticles (Fig. 2), the particle size in a separate layer is 10 and 20 nm, the thickness of an individual layer is determined using the formula (14), the thickness of the boundary layer is H = 0.5 µm << 1 mm.

For the inner area with the height 1 µm and diameter 10 µm, in which the charge density is distributed, a block unstructured tetrahedral grid is constructed, it is shown in Fig. 3. The grid consists of 16041 elements.

The charge density was determined using the formula (12) for the corresponding layer of particles. The boundary conditions for numerical modeling were chosen as follows: the value of the potential on the surface of a layer of particles with the size 10 nm – 0 V and 80 mV on the surface of a layer of particles with the size 20 nm. In this case, the change in potential occurs in proportion to the change in the porosity of the layer. On the lateral side of the selected area, the condition of zero electric field $\vec{n}\times\vec{D}=0$ is accepted. The required value of the dielectric constant is set in specific areas by using the formula (9) in accordance with the degree of compaction of particles inside the layer.

In the case of a micromodel, there considered not a layer of nanoparticles, but a large number of surfaces of nanoparticles falling into a given volume. The integer number of particles falling into a given volume is determined using the formula (6). For the inner area of the micromodel, an unstructured tetrahedral grid was built, it consists of 622595 elements. The surface charge density for nanoparticles in each layer is σ_{10} and σ_{20}, and the space charge density in the space between particles is determined as

$$\rho_{micro}=\frac{q_{10}+q_{20}}{2\left(V_{box}-V_{particles}\right)}, \quad (14)$$

where V_{box} is the volume of the corresponding layer, $V_{particles}=\frac{4}{3}\pi\cdot R_{10,20}^3\cdot N_{10,20}$ – volume occupied by the particles. The boundary conditions for the micromodel are chosen to be the same as for the macromodel.

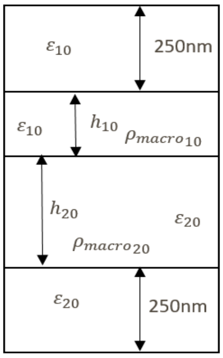

Fig. 2. Scheme of the macromodel.

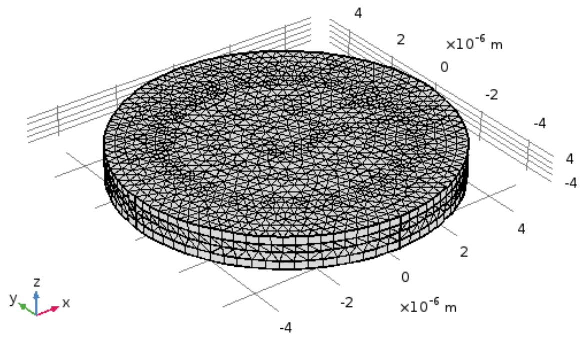

Fig. 3. Calculated grid of the macromodel.

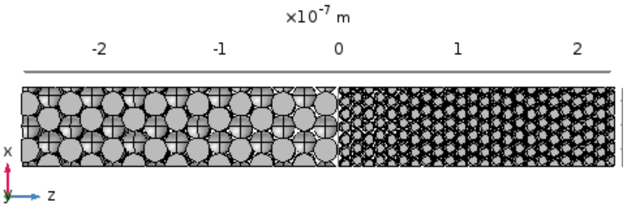

Fig. 4. Schematic representation of the geometry inherent to the micromodel.

Table. Input parameters of the macromodel.

Particle diameter, nm / Input parameters	10	20
h, nm	232.59	267.41
n_z	24	15
ρ_{macro}, C/m^3	–32.8	28.6
ε	2.8	3.9
P	0.58	0.45

4. Results and discussion

According to (13), for the macromodel, it is possible to determine the charge density in the contact area of the layers depending on the porosity of the particle layer as $\rho = \rho\,(P_{10}, P_{20})$. Similarly, the dielectric conductivity of the corresponding layer according to (9) also depends on the porosity of the layer. Therefore, it is advisable to consider the potential difference that occurs in the structure as a function of the porosity of the material.

For a numerical estimate, the following layer parameters were chosen: $d_{10} = d_{20} = 2$ nm, layer porosity $P_{10} = 0.58$, $P_{20} = 0.45$, respectively. Using the formula (13), it is possible to calculate the thickness of a layer of particles with the size 10 nm on the assumption that the entire thickness of the contact area of the layers and the charge are chosen so that the potential difference is not less than 100 mV. Based on expression (6), we can determine the number of particles in the layer volume. The input parameters for the model are listed in Table.

When going to a detailed consideration of interaction at the particle level (micromodel), it is necessary to set the charge density in the interparticle area $\rho_{micro20} = 426.81\ \mathrm{C/m^3}$, $\rho_{micro10} = 385.44\ \mathrm{C/m^3}$, as well as the charge on the surface $\sigma_{20} = \sigma_{10} = -1\dfrac{\mu\mathrm{C}}{\mathrm{m}^2}$.

The form of the potential distribution along the z axis (Fig. 4) for micro- and macromodels is shown in Fig. 5.

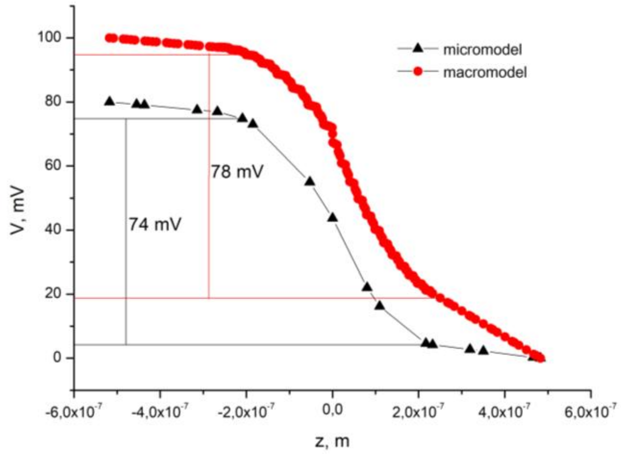

Fig. 5. Comparison of the potential distribution over the height of the model at the average charge density and detailed modeling of the surface charge.

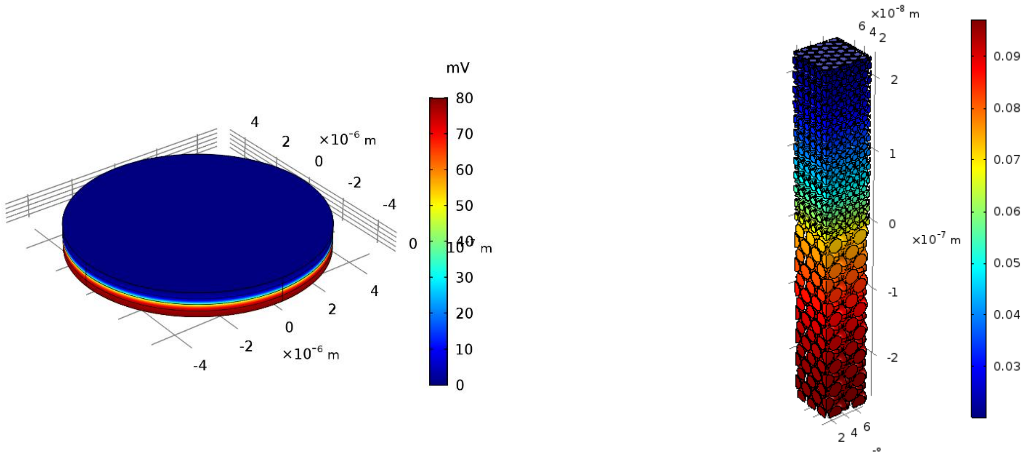

Fig. 6. Spatial view of the potential distribution in the macro- (a) and micro- (b) models.

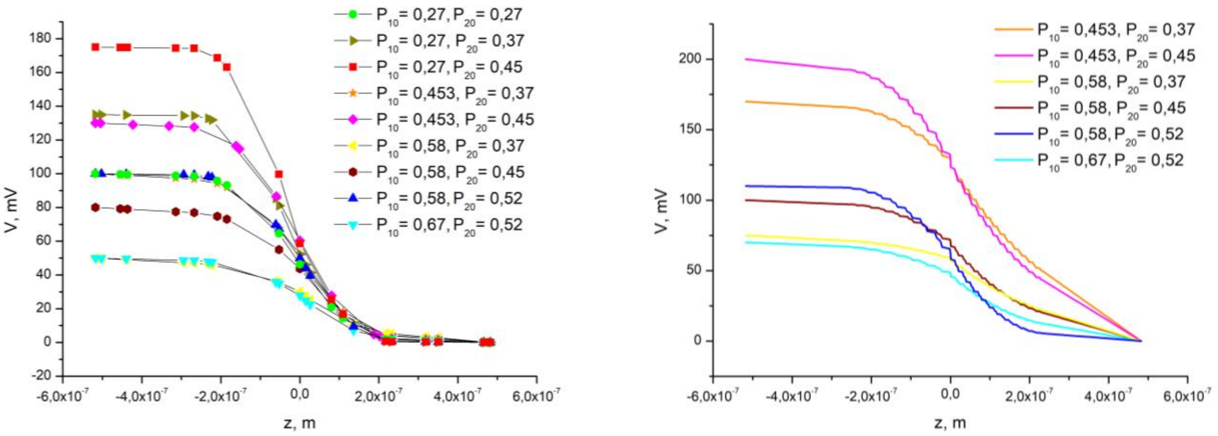

Fig. 7. Potential differences at different combinations of porosity of particle layers in the macro- (a) and micro- (b) models.

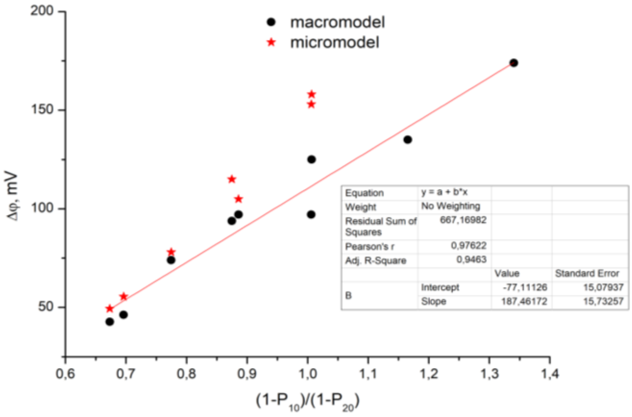

Fig. 8. Dependence of the potential difference on the ratio of the density of compaction of particle layers.

As can be seen from Fig. 5, for the potential calculated in the approximation of the micro- and macromodel, there is a small shift in absolute value, but the relative potential difference for both models is preserved.

Fig. 6 shows the view of the spatial distribution of the potential in the macro- (a) and micro- (b) models.

Fig. 7 shows the potential distribution with a change in the porosity of structures for both the macro- (a) and micro- (b) model.

As can be seen, the absolute value of the potential calculated in the micro-model approximation coincides with the analogous value calculated in the macromodel approximation, only in a certain range of porosity. This may be due to the influence of significant charge inhomogeneity at minimum values of porosity. In this case, an almost linear relationship is observed between the potential difference and the relative density of compacting the layers (Fig. 8).

5. Conclusions

Thus, the results of theoretical modeling of the electrostatic field in two-layer structures based on compacted nanodispersed hydrophilic oxide showed the possibility of creating a potential barrier in the hetero-interface area. The potential barrier in the heterointerface area appears during the adsorption of water in the entire structure due to differences in the density of surface states in layers with different particle sizes.

Also, the theoretical dependence of the bulk charge density in the contact area of layers of nanoparticles with different sizes on the porosity of the pressed structure has been obtained. The modeling was carried out in two ways: when considering the uniform distribution of space charge in the layers of particles, and also when considering the total surface charge for a large number of nanoparticles. For layers of nanoparticles, the potential distribution in this structure has been obtained for various values of porosity. The discrepancies in the estimate of the absolute value of the potential in the simulation by two methods increase with a decrease in the porosity of the structures, which indicates a significant inhomogeneity of the charge in these structures.

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Модель потенціального бар’єра, що виникає в гідрошарі, локалізованому у двошаровій пористій наноструктурі

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Анотація. Запропоновано модель потенціального бар’єра, який виникає у процесі взаємодії двох компактованих шарів, які складаються з наночастинок гідрофільного оксиду різного розміру у кожному шарі, при насиченні такої структури адсорбованою водою. Теоретично розраховано залежність густини об’ємного заряду пресованого порошкового матеріалу від щільності частинок у ньому. Отримано розподіл потенціалу по товщині контакта двох шарів, які складаються з наночастинок різного розміру.

Ключові слова: потенціальний бар’єр, двошарова пориста наноструктура, гідратований шар, наночастинка.