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CHANGE OF LOCAL CHARGE DENSITY BY CHANGE OF LOCAL MEAN CURVATURE IN BIOLOGICAL BILAYER MEMBRANES

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Abstract Highly positive curved parts of biological membranes show an increase in density of charge carrying molecules, while parts with less positive or negative mean curvature show a diminution. This has been shown by different investigators by marking the charge carrying molecules and examining the membranes by electron microscopy.

We here give an explanation for this finding based on electrostatics field theory. Assuming free lateral mobility of charge carrying molecules the membrane forms an equipotential surface. Under this premise the socalled charge simulation method can be used for building up computer models for the electrostatic properties of different shaped membranes. These models show the same behaviour for the charge density distribution as has been observed in the distribution of charge carrying molecules in membranes.

So simple electrostatic repulsion forces may also in biological membranes be the reason for local mean curvature related changes in charge carrying molecules distribution.

INTRODUCTION

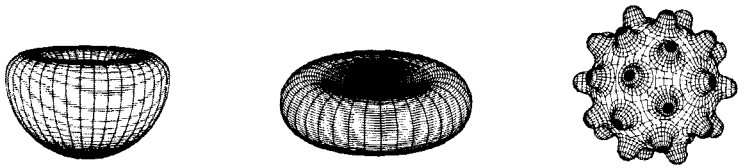
The core of every biological bilayer membrane consists of two sheets of different phospholipids mixed with colesterol. Fatty acid chains which contain no net charge and only small dipolmoments are directed towards the core, whereas head groups containing a net charge or at least a dipolmoment face towards the membrane surfaces. The lateral distribution of the different types of phospholipids in the inner and

outer part of the membrane is given by the resultant of the acting attractive and repulsive forces between the molecules.

In this presentation the influence of one of these forces, namely the electrostatic repulsion force between the charge carrying surface molecules will be examined. It is an a priori assumption that the bilayer is in the liquid crystal state, that no clustering occures, that all phospholipids and other membrane molecules are equally distributed in the plane.

This is in principle in accordance with results of electron microscopical examinations of biological membranes. One of the best studied is the erythrocyte membrane. For this membrane first MARIKOWSKY (1) showed that the charge carrying molecules in shape deviated erythrocytes namely echinocytes (Fig.1c) have a higher density on top of the protrusions (location of high mean curvature) than on the base (lowest mean curvature). Corresponding observations have since been reported by other investigators, examining different kinds of biological membranes.

MARIKOWSKY offers three explanations for this effect, all based on possible interactions between the charge carrying integral membrane proteins and the RBC 'cytoskeleton'. We here offer another explanation based on simple electrostatic field effects in connection with the shape related change in local mean curvatures of the membrane.



a. Stomatocyte b. Discocyte c. Echinocyte

FIGURE 1. Typical erythrocyte shapes used to build up computer models of the electrostatic properties of different shaped membranes are shown.

As basis for our model calculations we took shapes as to be found in shape altered erythrocytes. Fig. 1a shows a typical stomatocyte, Fig. 1b a discocyte and Fig. 1c an echinocyte produced by the program-system MOVIE.BYU on a VAX 11/780 using geometrical data (2,3) and procedures (4) from

the literature and our own experimental data . All these shapes are at least partly of rotational symmetry.

THEORY

According to the GOUY-CHAPMAN theory the electric potential in a charge carrying medium is determined by the POISSON-BOLTZMANN equation:

$$\Delta V = - \rho / \varepsilon$$

Because this equation is linear, a solution for a potential field with specific boundary conditions can be given by the superposition of particular solutions. The potential-field can be calculated as the sum of known potential fields which together fulfill the boundary conditions.

This is used by the so called charge simulation method (charge substitution) in electrical engineering to calculate the electric field strength of high-voltage equipment . Our program system* gives the opportunity to find an approximate solution for the electric field for any three dimensional boundary conditions of rotational symmetry even so there is no analytical solution (5).

Under assumption of free lateral mobility of charge carrying molecules we have to treat the membrane surface as an equipotential surface. This assumption is valid for a flat surface and also when the membrane will be locally bent.

To calculate the electrostatic properties of such a charge carrying membrane, an equipotential surface with given size, shape and total charge has to be modelled. This is exactly what the charge simulation method has been made for.

METHOD

Using the charge simulation method the inside and the outside potential field e.g. of a RBC model have to be determined separately. To calculate the outside field with the outer membrane surface as boundary condition the substitution charges (here point- and ring-charges o) have to be situated in the interior of the model. To introduce the membrane as boundary condition, contour points ■ with their

* developed at the Inst. für Allg. Elektrotechnik und Hochspannungstechnik, RWTH Aachen

potentials have to be introduced as to be seen in the upper right part of Fig. 2.

A matrix of potential-coefficients $\underline{p}$ has to be calculated which connects type and location of every substitution charge $\underline{Q}$ with the potentials $\underline{V}$ of the contour points.

$$\underline{V} = \underline{p} * \underline{Q}$$

The substitution charges can now be calculated. So there is a set of equations which gives an approximate solution of the field outside of the contour points. If this approximation is good enough any electrostatic property of this configuration can be calculated. Here we are interested in the surface charge density on the boundary, which is given by

$$\sigma = \text{Div } \underline{D}$$

An example of an electrode of rotational symmetry in vacuum shaped like a discocyte (Fig. 1b) is shown in the upper right part of Fig. 2. The outside membrane is simulated. The graph in Fig. 2 shows the big variation in surface charge density along the outline of this electrode.

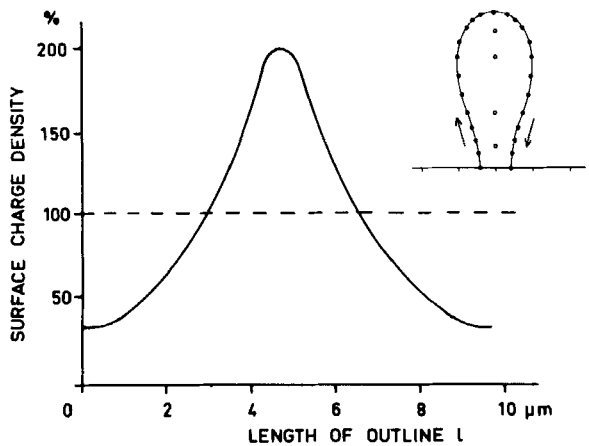


FIGURE 2. Surface charge density along the outline of the model of a discocytic shaped electrode (Fig. 1b) computed by the charge simulation method (upper right part: substitution charges o, boundary points ■).

RESULTS

The upper part of Fig. 3 shows the change in surface charge density along the outline of computer simulated stomatocytes of rotational symmetry. The charge density along the outline of three similar stomatocytes with increasing depth of the dimple (Ø.8µm to 1.5µm) from a to c are given, each of the same volume, surface area and total amount of charge.

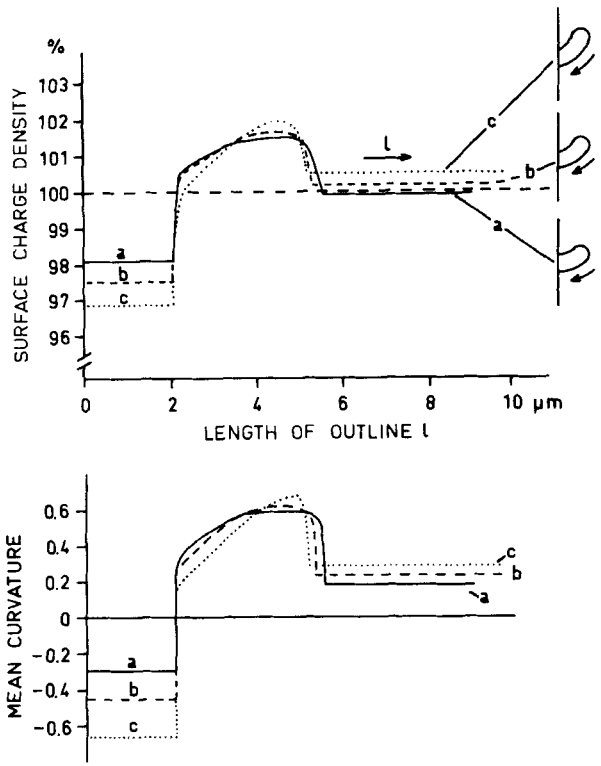


FIGURE 3. The surface charge density along the outline of stomatocytes with increasing depth of dimple (a-c upper part). The graphs in the lower part give the related local mean curvature.

The related graphs of the local mean curvature in Fig. 3 lower part show the coincidence in decrease and increase of mean curvature on the one hand and charge density on the other. With increasing depth of dimple, which means increase

in local negative curvature, there is a local decrease of charge density inside this dimple.

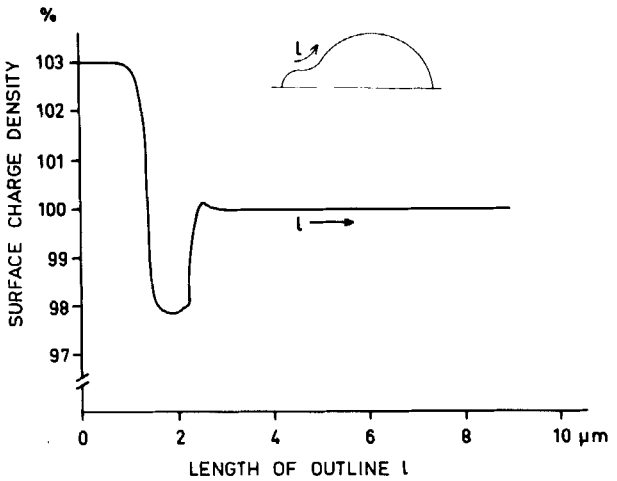


FIGURE 4. The surface charge density along the outline of a big sphere with one small protrusion is given as a simple model for an echinocyte (fig.1c).

Fig. 4 gives an approach to the electrostatic properties of an echinocytic RBC shape. A big sphere with one protrusion has been simulated. Here the highest charge density is on the top of the protrusion (mean curvature 1 μm^{-1}) while the bottom of it has even less charge density than the main body. This is again in parallel to the change in local mean curvature. The base of the protrusion is the locus of lowest mean curvature ($0 \mu m^{-1}$) because one of the two main curvatures here becomes negative.

DISCUSSION

Fig. 2 shows for an electrode in vacuum the clear relation between change in mean curvature and surface charge density in every point of the surface. This holds in principle for space charge carrying media. Fig. 3 shows, that under the same boundary conditions a variation in shape (here as increasing stomatocytosis of RBC) which is related to the increased variation of curvature gives a similar increase in variation of surface charge density.

Nevertheless, variation of density in vacuum is much more intense because there are no covering effects by freely mobile ions. In common RBC shapes in vacuum (ionic strength 0 Mol/L) there is a change in surface charge density of several hundred percent (Fig. 2), for a ionic strength of 10^{-4} Mol/L of several percent (Fig. 3 and 4) and for 10^{-1} Mol/L of some 0.1 percent (not shown).

There is no direct proportional relationship between curvature, surface charge density and ionic strength. The local charge density depends not only on the local mean curvature, but also on the distance of the surrounding charges and this the more the lower the ionic strength is. So there is an asymmetry in the behaviour of change in surface charge density related to change in mean curvature which is due to the steric differences of the surroundings.

Fig. 4 shows that there is a qualitative agreement between model and the observations made by electron microscopy even so the variation in surface charge density seems to be smaller in the model. This is due to the small differences in curvature which have been used here to get a clear model. Also there may be local changes in medium properties, e.g. ionic strength, which increases locally the electrostatic influences on the charge carrying molecules.

CONCLUSIONS

There is an influence of local mean curvature on charge carrying molecule distribution inside and outside of a membrane. Those parts of the surface with local mean curvature higher than the surroundings display a correspondingly higher charge density, while a lower mean curvature leads to a lower charge density.

So the well known physical laws describing the electric field give an explanation for the observed variation in density of charge carrying molecules depending on variation in local mean curvature.

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