MODELING THE STRUCTURE OF HEMOGLOBIN APPLYING A DIELECTRIC METHOD FOR MONITORING THE STATE OF BIOLOGICAL OBJECTS

Batyuk L.V., Kizilova N.N.

Kharkiv National Medical University, Kharkiv, Ukraine
PoreLab, Department of Chemistry, Norwegian University of Science and Technology, 7491 Trondheim, Norway

The region of dielectric relaxation of water molecules in blood cells or human tissues at a frequency between 1 Hz and 50 GHz is most interesting for obtaining unique information on the fundamental properties of liquids, on the molecular structure of proteins, on the dynamics of changes and orientations of liquid molecules with temperature and composition variations [1-2]. Using the values of the complex permittivity measured in this region, we can calculate the static and optical permittivity and relaxation times, which are related to the order parameters: the average correlation factor between the molecules and the change in activation entropy [3]. At the same time, the reliability of the conclusions about the supramolecular structure of a protein or changes in its structure depends to a large extent on the choice of the density of frequency points and the accuracy of measurements, the choice of an adequate model of dielectric relaxation measurement and the possibility of conducting temperature and concentration studies that reflect the formation of a supramolecular structure.As an object and model of the study, we have selected hemoglobin of erythrocytes. This choice is due to the possibility of using the object as a sensor that responds to changes in the state of the body, as well as for testing the created measuring tools, since the electrophysical characteristics of hemoglobin are presented in many literature references [4-5]. Protein models are characterized by a loose packing of atoms. This may affect the calculation of depolarization coefficients. An algorithm was developed for filling the hollow parts of model objects for a more accurate calculation of the depolarization coefficients with liquid. The algorithm is based on the fact that only the internal cavities of objects are filled without increasing its geometric dimensions. To consider have took an ellipse. In solving this problem, resonant methods for measuring the permittivity spectra were used. When processing the results, the basic principles of mathematical statistics, numerical methods of approximation, optimization of functions and solving systems of linear algebraic equations were used.The structure of the proposed model allows for its parametric identification with almost accurate reproduction of the dynamics of the distribution of dielectric relaxation in the concentration-temperature space, which indicates the restructuring of the liquid structure in these temperature ranges. The presence of the dual effect of water on the structure of hemoglobin leads to the fact that the change in free energy during protein denaturation is 15-17 kcal/mol with a total energy of hydration on the protein macromolecule of the order of 102 kcal/mol. It turned out the adequacy of this model is maintained even if it is simplified by increasing the degree of aggregation of red blood cells. This process indicates a restructuring of the water structure surrounding the hemoglobin molecule and is explained by the formation of cluster-type water regions.

Reference

1. Chelidze T. Dielectric spectroscopy of blood // J. of NonCryst. Solids. 2002. Vol. 305. P. 285–294.
2. Batyuk L.V., Kizilova N.N. Novel monitoring system for quantitative estimation of efficient medical treatment of diseases // Bull of V. Karazin Kharkiv National University. 2019. Vol. 43. P. 4–10.
3. Batyuk L.V. Influence of cancer disease on dielectric characteristics of structural-functional state of erythrocyte membranes // Medical Science Journal. 2015. Vol. 74. P. 11–17.
4. Батюк Л.В., Берест В.П. Evaluation of relaxation frequency of hemoglobin // Медична та клінічна хімія. 2019. Т. 21, № 3. С. 17–18.
5. Salamon Z., Macleod H.A., Tollin G. Surface plasmon resonance spectroscopy as a tool for investigating // Biochim et biophys acta. 1997. Vol. 1331. P. 131–152.