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Preliminary study on the estimation of complex permittivity for biomolecules with molecular simulation under the application of electric field in the millimeter wave frequency range

Takuto Sugino*(1), Shun Ding(1), Kensuke Sasaki(2), and Yukihisa Suzuki(1)
(1) Tokyo Metropolitan University, Tokyo, Japan, e-mail: sugino-takuto@ed.tmu.ac.jp; ding-shun@ed.tmu.ac.jp; y_suzuki@tmu.ac.jp
(2) National Institute of Information and Communications Technology, Tokyo, Japan, e-mail: k_sasaki@nict.go.jp

Biological tissue has its own complex permittivity. Measurement of the complex permittivity of biological tissue has been conducted in many studies, however it is a macroscopic level study. On the other hand, when evaluating electromagnetic field exposure for the cell scale, data on the complex permittivity for the molecular level is required. The purpose of this study is to establish the scheme to estimate macroscopic complex permittivity of bio-molecules from microscopic molecular simulations. If the complex permittivity is obtained from theoretical simulation, induced electromagnetic fields within biological-cells will be predicted, and it helps to discuss possible effects of electromagnetic field on the biological systems.

As a preliminary study, the method of estimating complex permittivity is considered with molecular simulation. Simulation is performed using molecular simulation software MOE ver. 2018.01 (CHEMICAL COMPUTING GROUP INC.) whose calculation engine is NAMD ver.2.12 (Theoretical and Computational Biophysics Group and the Parallel Programming Laboratory). The possibility to estimate the complex permittivity for molecules in the millimeter wave band is investigated with data obtained by computer simulation. Since biological-cells contain more than 1000 types of organic molecules [2], it is expected to be difficult to estimate all types of complicated molecules by simulation. Therefore, in the beginning of this study, simple molecules such as KCl, $MgCl_2$, $LaCl_3$ are examined. Figure 1 and 2 show the dependence of the location of K ions and Cl ions on the time as the simulation results when an electric field of 160 GHz is applied to KCl molecules.

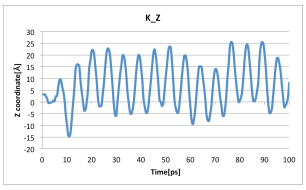

Figure 1. simulation result (potassium ion)

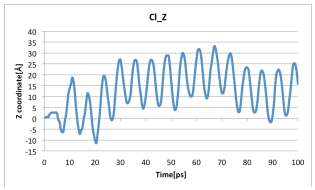

Figure 2. simulation result (chloride ion)

Estimations of conductivities for biomolecules are carried out by using data obtained from simulation with the method described in literature [1]. Initially, instantaneous current is obtained by equation (1) based on the results of molecular simulations.

$$I(t) = \frac{1}{\Delta t L} \sum_{i=1}^{N} q_i [z_i(t + \Delta t) - z_i(t)] \tag{1}$$

where, z_i is the coorsinate parallel to the direction of applied electric field vector, q_i is charge of the atom i, L is the size of the simulation region, N is the number of the atom given in the simulation, t is the time, and Δt is the time interval used to record the data. Conductivity is calculated by using the current and applied electric field obtained here. We will report on the estimation of complex permittivity derived from this method for not only simple molecules mentioned above but also basic biomolecules such as lipid which are the basis of cell membranes.

1. Carles Calero, Jordi Faraud, and Marcel Aguilella-Arzo, "Molecular dynamics simulations of concentrated awueous electrolyte solutions" *Taylor & Francis*, 37(2011), pp.123-134.

2. K.Nakamura, A.Fujiyama, and K.Matsubara, trans. " *Essentioal Cell Biology : An Introduction to the Molecular Biology of the Cell*," Tokyo, nankodo, 1999.