

DIFFUSIONAL AND HEAT MOTION OF LIPID MOLECULES IN BILAYER MEMBRANES

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As a rule diffusion constant (DC) is calculated on the base of molecules mobility investigations in a macroscopic timescale. It's caused by aspiration for accurate measurement of DC, because in the long timescale molecules displacement is greater, so it can be defined more precisely. However, it's rather obvious that DC value should be in close relation with parameters of molecular heat mobility. Direct experimental investigation of individual molecules mobility can not be accomplished, but it is possible to get all its parameters from a molecular dynamics (MD) simulation. In this work we've calculated DC from MD simulation of heat mobility.

For MD simulation we used opls-based model of a fragment of DSPC lipid bilayer in water (48 DSPC/1759 waters). For MD calculation GROMACS with integrator sd was used, time step for integration was 0.25 fs and cut-offs were 1.5 nm. Length of all trajectories was less or equal to 100 ps. All parameters of equilibrated model were in a good agreement with parameters of real bilayer.

We've considered "effective diffusion constant" (EDC), ratio between squared molecule center of mass (COM) displacement and time period of this motion. If this period is small EDC has a non-monotone time dependence and with time it becomes a DC. If the timescale is less than a period of molecules thermal vibrations, COM movement between two walls of potential hole can be approximated by a linear subsection. If we suppose that thermal vibrations are harmonic, in the timescale by order of magnitude equal to the period of this vibrations the average COM displacement will not be a function of time. In the greater timescales the diffusional drift of equilibrium point of heat vibrations becomes noticeable. Our description of this motion is based on the solution of 2D random walk problem. Time dependence of EDC in all timescale range was defined as a sum of described above three dependencies multiplied by corresponding exponential functions which synthetically managed to display appearance and attenuation of these functions in different timescales. After fitting of the MD data by the received dependence we've found that there are a considerable mismatch near 1–10 ps. This mismatch was completely removed by a proposal that directions of single diffusional movement are not equally possible. As a result a model derived curve coincide with the MD data ($RMSD \sim 0.01$) and with time it tends to the limit which coincides with a real DC for DSPC ($2.86 \cdot 10^{-8} \text{sm}^2/\text{sec}$). Moreover, we showed that probability of diffusional displacement in the direction of antecedent displacement is three times greater than in the opposite direction.

So, it was shown that DC value could be calculated on the base of heat molecular motion parameters in a short timescale (< 100 ps). Moreover, it's impossible to separate pure diffusional and vibrational movements. All diffusional displacements have features of vibrational movements.