SIMULATION OF THE MAIN PHASE TRANSITION KINETICS IN THE LIPID MEMBRANES

Sizonenko T.O., Kharakoz D.P.

Institute of Theoretical and Experimental Biophysics
142290 Pushchino, Moscow region, Russia. Tel.: (4967)73-93-82.
E-mail: LuckyDevil2007@gmail.com

This work is in the scope of studies developing an earlier formulated idea about the phase-transitional mechanism of synaptic exocytosis. According to this idea, the exocytosis is driven by Ca^{2+}-induced solidification of cytoplasmic membrane (main phase transition). The idea presents a novel view of a range of unsolved biophysical and physiological problems related to the mechanism of functioning of chemical synapses. Present work deals with mathematical modelling of main phase transition aimed at clarification of its kinetic features. Transition rate is determined by the probability of new phase nucleation and by the speed of new phase propagation. These factors depend on the temperature and the inclusions in the membrane, which may serve as a pre-existing seed new phase.

The transition kinetics is modelled by Ising model on triangle lattice, with kinetic Monte-Carlo method. Each point is occupied by a lipid chain. Every chain can exist in two states corresponding to gel or liquid crystal. The energy of neighbour interaction, transition rate constant and size of the system are among the important parameters of the model. The thermodynamic and kinetic parameters have been calibrated by comparing theoretical results with the experimental acoustic and calorimetric data on main transition in artificial membranes.

With reasonable assumptions about calcium effect on phase transition, we estimated that the solidification time for the synaptic membrane is comparable with the known synaptic delay in fast synapses. Membrane heterogeneities, able to reduce the energetic barrier, strongly enhance the probability of the transition. Thus the probability of exocytosis and, hence, of synaptic transmission can be managed by the heterogeneities in synaptic membrane.

References

1. *Kharakoz, D.P.* Phase-Transition-Driven Synaptic Exocytosis: A Hypothesis and Its Physiological and Evolutionary Implications // *Biosci. Rep.* **21**, 6, 2001.Pp. 801–830.