**Abstract**

In this thesis, we construct computational models and consider one possible scenario of chemical evolution in which the life generates from chemical reactions among inorganic matters. In particular, we pay attention to structure and function of primitive membrane and the possibility of membrane evolution.

There have been mainly two types of researches concerning the origins of life. One of them is the constructive experiment in which they synthesize organic matters from inorganic matters artificially in laboratory and they seek how the life can be synthesized. The other one is the theoretical study in which they find the relations between chemicals which are modeled abstractly and they seek how the life exists as a system. The former is the reductionism, on which they consider the structure of meterials as the most important property of life, based on the structure of materials. On the other hand, the later is the holism or the system methodological stance on which they consider the relationships among materials as the essense of life. The two above are totally different ways of looking at the life. It is, however, important that we consider the two approaches in order to research the life which is based on not only materials but also on complex chemical interactions. Nonetheless, there is little discussion about methodologies to integrate the two ways. Although the former way is based on the reductionism, it is also a constructive way because an organic molecules are synthesized in a laboratory. The later is based on the holism but also it is constructive because systems are constructed from the relations among materials. In this thesis, we attempt to combine the two stances, material reductionism and system methodological holism, by constructive approach and suggest a new method to investigate the origins of life.

We consider the chemical evolution from the standpoint on which inorganic materials also evolve into the life by natural selection. Some functions related to the natural selection are necessary for the materials to evolve. In other words, we must take both structure and function of matrials into account to consider the chemical evolution. In this thesis, we in particular pay attention to the structure and function of primitive membrane. The

reason comes from the facts that the amphiphilic molecules which can self-assemble into membrane, that the evidences of the molecules existing on the primitive earth have already been found, and that the membrane has functions of adsorption and permselectivity.

From the standpoint of material structuralism, we analyze conformation and self-assembled structure of amphiphilic molecules by molecular dynamics method. The current cell membrane is formed of bilayer structure in which hydrophobic part of amphiphilic molecules are faced inside each other. The size of vesicles which is made of amphiphiles is assumed from nano-meters to micro-meters scale. Although, in usual molecular dynamics, each atom is modeled and interactions among atoms are defined and calculated, it takes too long time to calculate them by the current computer systems. In this thesis, we use a coarse-grained approach in which some of atoms are modeled as one super-atom and it can be within reach to calculate micro-meters order structure. As a first step, we model simple amphiphilic chain polymers as coarse-grained and simulate them in order to prove availability of the coarse-grained model for amphiphilic molecules.

Second, we construct a coarse-grained model of phospholipids which are widely used in current cell membrane. Then, surface adsorption and membrane absorption as functions of membrane can have an effect on resolve the concentration problem which is one of major problems in the origins of life. The concentration problem is a problem to ask how the high concentration state of small organic molecules is sustained in the prebiotic condition. We propose a more specific problem on this concentration problem: Can phospholipids maintain the bilayer structure, adsorb and absorb amino acid molecules, and concentrate them under high pressure and high temperature condition such as hydrothermal vent? And we show the possibility by constructing a coarse-grained model of phospholipids and amino acids and by simulating them. The results show that it is possible for lipids to maintain the bilayer structure and to adsorb and absorb amino acids, and to concentrate them even if it is under high pressure condition. The adsorption and absorption can influence the stability and the permeability of the membrane. The linkage from the structure of membrane to the function is provided from the model.

Next, from the results above, we investigate how the membrane permselectivity can influence the evolution of proto-cells. We propose an abstract proto-cell model, an autopietic

cell model, in which there is an auto-catalytic reaction cycle inside and the membrane substances are produced from the cycle, and we show that the possibility of diversification can occur by the membrane permselectivity. The results show that the size of cells can vary depending on the membrane permselectivity even if it is the same initial condition and parameters. The view from the function of membrane to the evolvability of proto-cells is provided from this model, and the sufficient conditions of the diversification are also provided. Specifically, we show two sufficient condistions. One of them is that the change of chemicals inside a cell and the total amount of inflow and outflow are highly correlated, and the other one is that the probability of concentration changes inside a cell is low. And we discuss that the conditions depend on the property of auto-catalytic reaction cycle and on the pattern of membrane permselectivity. We furthermore attempt to propose a new scenario about the diversification of proto-cells driven by membrane permselectivity on the working hypothesis as an assumption which comes from the simulation results.

Last, we conclude that the membrane structure is important in the chemical evolution because the membrane has the fuction of concentrating the small organic molecules on and inside itself and influences the diversification of cells, and that the membrane itself can evolve as an unit of natural selection. We claim in this thesis that the integration of reductionism and holism can contribute to finding new knowledge about the life system. In particular, we suggetst that the constructive approach is often useful for studies, such as an analysis of the mutual and complex interactions among many elements, or an analysis of systems which no more exists in this world like chemical evolution.