compared. These potential energy functions were derived from the probability distribution function of its tetrameric step conformations calculated from trajectories of MD simulations of free DNAs which include all 136 types of tetramers. This gave good agreement with some experimental results, but shortage of structural sampling made the accurate estimation of distribution function difficult. In this work, we estimate the probability of occurrence of each tetrameric step sequence on given tetrameric step conformation using a Bayesian approach using the same structural dataset. We apply this approach to known protein-DNA complex structures, and assess the performance of predicting the sequence region where indirect readout makes important contribution to the binding affinity.

2P-089 DNA ブランチマイグレーションの反応速度予測に向けて Towards the prediction of kinetics of DNA branch migration

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We propose a model to predict the kinetics of DNA branch migration based on the nearest-neighbor model. A branch migration is a DNA chemical reaction where a single strand extends its base pairing with its complement and then removes the competitive strand from the duplex. This branch migration process plays an important role in a living body. For example, a structure of a holiday junction is controlled through this branch migration reaction. Furthermore, the branch migration is utilized to various applications using DNA. Recently, Seeling *et al.* succeeded in the construction of enzyme-free logic gate by DNA. Seelig's logic gate receives a single-stranded DNA as input and outputs another single-stranded DNA. The driving force of this logic gate is only hybridization and branch migration. The branch migration is used to transform from input into output. Moreover, on the basis of Seelig's logic gate, we also developed new DNA logic gate, called DNA comparator. These efforts enable us to implement an autonomous molecular logic gate without any enzyme. Thus, the importance of branch migration reaction grows day by day not only to analyze the biochemical reaction but also to construct attractive artificial molecular systems. However, so far, the kinetics of branch migration cannot be predicted accurately. The kinetics is one of the most important parameter in order to design the logic gates driven by branch migration. In this presentation, we propose a nearest-neighbor model to predict the kinetics of DNA branch migration from its DNA sequence. To this end, we focus on the fact that the branch migration is regarded as the probabilistic random walk depending on its DNA sequences next to the branching point. We will present our latest results to verify the applicability of our model by fluorescent experiments.

2P-090 DNA 分子で作られた二次元結晶の成長メカニズムの解明 Elucidation of growth mechanism of two-dimensional crystal created by DNA molecules

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In the field of nanotechnology, one of major goals is to measure physical properties of molecules or nanoparticles ordered at mesoscopic level. In order to achieve the goal, a method which can control the position of the materials at nanometer level must be developed. Nanostructures created by DNA molecules have the possibility as molecular scaffolds to arrange the materials on nanometer scale. DNA double-crossover AB-staggered (DXAB) tile is one of DNA nanostructures. DXAB tiles can self-assemble into two-dimensional (2D) periodic DNA tile arrays that are grown into micrometer size. We aim to elucidate a growth mechanism of 2D DNA tile array and to control the size and shape of 2D DNA tile array. Therefore, we required statistical evaluation of the size and shape of DNA arrays in order to ascertain the factors that are effective in the crystal growth of DNA tiles. However it was difficult to observe the micrometer-sized 2D DNA arrays by Atomic Force Microscopy (AFM) because AFM specialized in nanometer-scaled observation. Therefore, we applied the optical microscopy with fluorescent probe in order to observe the micrometer-sized DNA arrays. The shape of DNA array was a filament-like structure and the size of DNA array was ca. $8 \mu\text{m} \times 1 \mu\text{m}$ on average. We are now going to examine the relationship between various factors and the structure of DNA tile arrays in detail.

[1] M. Tagawa, K. Shohda, K. Fujimoto, T. Sugawara and A. Suyama, *Nucleic Acids Res.*, 35, e140 (2007)

2P-091 時間分解蛍光分光を用いた逆ミセルに入れたタンパク質の水和水のダイナミクスの研究

Study of the dynamics of hydrated water of protein in reverse micelle using time-resolved fluorescence spectroscopy

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It is considered that hydrated water plays an important role in functions and structural fluctuation of protein. The purpose of our research is to study the dynamics of the hydrated water in the time range from femtoseconds to

nanoseconds as a function of the number of water molecules surrounding a protein. Molecules in solution electronically excited by light absorption show the energy relaxation process due to the configuration change of the surroundings of the molecule while it emits fluorescence due to population relaxation from the electronic excited state to the ground one. The fluorescence spectrum shifts to the low-energy side with time, and so we can study the dynamics of the surroundings of the fluorescent molecule by observing the time-dependent shifts. We use a sample of a dye molecule trapped in a hydrophobic pocket of a protein confined in a reverse micelle. It is possible to control the size of reverse micelle on a nanometer scale by adjusting the molar ratio of water to surfactants, and so we can control the number of the surrounding water. Because the dye molecule interacts with the surrounding water, the dynamics of the hydrated water will be studied by time-resolved fluorescence spectroscopy of the dye molecule. Coumarin dyes and bovine serum albumin are used as a dye molecule and protein, respectively. A reverse micellar solution is prepared with a surfactant of sodium bis(2-ethylhexyl) sulfosuccinate (AOT) and a solvent of isooctane. Time-resolved fluorescence spectroscopy is done by a method of time-correlated single photon counting with time resolution of a few hundred picoseconds and by femtosecond time-resolved fluorescence up-conversion technique.

2P-092 塩の溶媒和効果が誘起する水/有機溶媒混合系の階層的秩序 Multi-lamellar structures induced by hydrophilic and hydrophobic ions added to a binary mixture of water and organic solvent

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Solvation effect plays an important role in various field of natural science. One of the most interesting issues is its influence on the mixture of water and organic solvent. Recently, we examined the effect of NaBPh₄, which is a kind of salt composed of hydrophilic cation Na⁺ and hydrophobic anion BPh₄⁻, on the phase behavior of the mixture of D₂O and 3-methylpyridine (3MP).

By optical microscope, a number of droplets with a size of $10 \mu\text{m}$ were observed at room temperature when 85 mM of NaBPh₄ is dissolved in the mixture of D₂O and 3MP. These droplets showed maltase cross patterns at a condition of crossnicole, using polarized light. On the other hand, only homogeneous view within whole sight was observed above 318 K. The maltase cross patterns are known to be observed when the system forms the multi-lamellar vesicles. In order to verify the detailed structure of this system, we have carried out small-angle neutron scattering (SANS) experiments. At lower temperature below T = 318 K, a sharp Bragg peak is observed together with second and third peaks. This profile is interpreted as a lamellar structure. On the other hand, a single broad peak is observed above T = 318 K, suggesting to form a disordered structure. These results show that a lamellar/disorder phase transition occurs with elevating temperature, which is similar to the case of mixtures of water/oil/surfactant.

2P-093 α シェイプを用いた蛋白質分子内空洞の探索プログラムの作成 An application program by using alpha-shape method for searching voids of a protein

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Some protein molecules, which have functions in aqueous solution, have voids in interior of the molecules where water molecules can enter. Accessible surfaces of proteins for water molecules can be regarded as small walls at atomic scale. Brute-force algorithms for searching such voids by dividing 3-D space into small cells have merits in computational time with parallelization of calculations. But these algorithms lose the information of the topologies which is made of closest atom-pair connections through space. On the other hand computational geometry methods have advantages in quantitative calculations by using the topologies of the atom-pairs. In this work, we have made the programs for searching voids in a protein with alpha-shape method in computational geometry in order to utilize them for other scientific computational programs for proteins which use protein surface topologies calculated by the alpha-shape method, e.g. extended scaled particle theory (hydration free energy calculation) [1] and boundary element method (electrostatic field calculation of protein surfaces). We have made whole parts of the application programs by ourselves, in the manner of structured programming. Two proteins, bovine pancreatic trypsin inhibitor (BPTI) and Protein G, were used to check our programs. Our application programs enabled us to find small voids which are made of few isolated water molecules in interior of BPTI. If water molecules are not identified in the voids with the X-ray structure of a protein, these voids usually cannot be found by bare-eyes with sliced pictures of proteins by computer graphics. In our presentation, we also mention our 3-D stereoscopic visualization of voids by using virtual reality method [2]. 1 M. Irisa, *et al.*, *J. Mol. Liq.* 65/66, 381 (1995) 2 M. Irisa, *et al.*, *Biophysics* 3, 57 (2007)

2P-094 蛋白質の熱容量温度依存性と水の状態方程式の関係 Heat capacity changes of protein and the equation of state of water