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テラヘルツ時間領域分光法による生体分子ダイナミクスの研究

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The terahertz time-domain spectroscopy (THz-TDS) is applied to the measurement of the delocalized vibrations which are conventionally investigated by the incoherent neutron scattering. The delocalized vibrations of the proteins with biochemical activities involve the anharmonic motions which are the fluctuation between conformational sub-states. The anharmonic motions are observed by the sharp increase of the average mean squared atomic displacements with temperature. The onset of the anharmonic motion requires the sufficient level of the hydration and a temperature above 200 K. Water molecules play an important role for the anharmonic motions of proteins with biochemical activities. Therefore the relation between the hydration and the anharmonic motions of biomolecules needs to be investigated. We have conducted the THz-TDS of the various biomolecules, which includes amino acids, short peptides, and proteins, focusing on the hydration. In the studies of amino acids and short peptides it is suggested that water molecules stimulate the rearrangement of the biomolecules which results in the conformational changes or the significant decrease of the inhomogeneity in the molecular structure. In addition to the interaction between water molecules and small biomolecules, which provide the information about motions of side chains, the hydration effects for the protein dynamics have been investigated with the THz-TDS.

K. Yamamoto, M. Yamaguchi, M. Tani, and M. Hangyo : Studies on Biomolecular Dynamics with Terahertz Time-Domain Spectroscopy

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広帯域誘電分光による水/生体高分子ダイナミクスの研究

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Dielectric spectroscopy is a conventional experimental technique to study molecular dynamics of complex systems like biological systems. Recent developments on broadband dielectric spectroscopy (BDS) make it possible to observe dielectric relaxation processes in a wide frequency range from 1 μ Hz up to 30GHz, and BDS is now applied to fundamental and applied studies in various fields. Details in other measuring systems available in higher frequency region with narrow bands are not treated in the present talk. Biological molecules show various modes of dynamics with different relaxation times in the wide frequency range. Water with the relaxation time of 8ps at 25 $^{\circ}$ C is interacted by biological molecules and shows the slow dynamics. Though molecular behaviors are complicated by also ions, the relaxation mechanism determined by interactions between water and biological molecules has been understood for some cases. Details in principles, recent developments and typical examples of BDS studies will be explained.

S. Yagihara : Broadband dielectric study on dynamics of water/biomolecules

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ラマン散乱からみる生体高分子ダイナミクス

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Raman spectroscopy is one of the important tools to obtain the experimental information on large amplitude modes of biomacromolecules. The low-frequency Raman spectra of two protein crystals, a tetragonal crystal of lysozyme and a hexagonal crystal of BPTI, and DNA films are shown in Figure 1. There are the central component and broad bands with several humps. The spectra were fitted by the sum of relaxation modes and damped harmonic oscillators[1]. The central component reflects the relaxation times of water molecules. On the other hand, the broad bands are attributed to intramolecular vibrations. One characteristic mode (S-mode) around 20 cm⁻¹ of DNA films sifts coupled with the A-B transformation. The phonon whose origin is common to S-mode was observed in Raman spectra of nucleoside and nucleotide crystals. Based on the analysis of MD simulations of guanosine dihydrate, we propose that the origin of this mode is to be the translational vibration of stacked bases. [1] H. Urabe et al., Biophys. J. 74, 1533(1998).

Y. Sugawara and H. Urabe : Dynamic behavior of biomolecules monitored by Raman spectroscopy

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細菌べん毛の構造形成と作動原理

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細菌べん毛は約25種類のタンパク質が、それぞれ数コピーから数万コピー集合して組みあがる超分子ナノマシンである。大きく分けて、基幹部、フック、繊維の3つの部分構造からなる。基幹部は直径約30nmの高速回転モータとしてトルクを発生する。繊維は直径約20nm長さ10数 μ mにもなる細長いらせん型のチューブ構造によりスクリュープロペラとして推進力を産み、細菌の直線的な泳ぎや方向変換を駆動する。フックは両者を連結する長さ約55nmの短く曲がったチューブ構造で、曲げに柔軟くねじれに強い構造によってユニバーサルジョイントとして機能し、時々刻々、運動パターンに応じて様々に向きを変えるプロペラにトルクを伝える。反転頻度制御機構つき回転モータと、モータ反転時に繊維の根元に生じるねじれ力によってらせん構造を左巻-右巻きと切り替えることのできるプロペラが、細菌の走行行動を支えている。基幹部は細胞膜を貫通して固定されており、その細胞質側にはべん毛特異的タンパク質輸送装置が結合し、9種類の軸構造構成タンパク質、3種類のキャップタンパク質、それに発現制御や長さ制御に関わるタンパク質を2セットに分けて、べん毛中央を貫通する細長いチャネル内へ順次輸送する。べん毛先端に輸送されたタンパク質はその自己集合能により先端の構造を認識して、キャップ構造の助けを借りながら、結合すべき構造であれば組み込まれて構造の一部となりべん毛構築を進めるが、そうでなければ細胞外へ分泌される。X線回折法や電子顕微鏡像の画像解析法による立体構造解析や遺伝学的機能解析を組み合わせることによって、べん毛各部の自己構築、構造スイッチ、長さ制御などの仕組みや、しなやかさと高精度を併せ持つ生体超分子ナノマシンの設計原理が明らかになりつつある。

K. Namba : Molecular mechanisms of self-assembly and switching of the bacterial flagellum