1P054 単粒子解析のための粒子投影方向決定の手法—シノグラムライン特徴量とその応用
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A novel method to determine Euler angles for single particle analysis : Sinogram-line features and its apprication
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Ab-initio orientation determination for 3D reconstruction in single particle analysis from electron micrographs requires finding a sinogram line pair with the same intensity distribution, i.e., the same features. Conventional sinogram correlation method is often employed, but is costly in calculation time and is too sensitive for noise. We, here, propose that the similarity of a pair of sinogram lines is measured as the distance between two points representing the sinogram lines in six dimensions of feature space. Some tests were submitted to compare the new method with correlation method using a set of projections from myosin head (1VOM, S/N=1). These results show that only six features should indicate the similarity of the lines better than the conventional correlation even under the noise-containing conditions. Furthermore, the calculation speed and the computer resources by the feature-based method are 1/17 larger than those by the correlation method. These advantages become outstanding when the methods are applied to iteration process like simultaneous common line determination. We here show the comparison between feature-based method and the correlation method and explore possibilities of application of the new method to Euler angle determination.

1P056 トップエントリー型極低温電子顕微鏡を用いた電子線トモグラフィー法における最適撮影条件の探索に関する研究
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Optimal conditions for electron cryotomography with liquid helium-cooled specimen stage
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Electron cryotomography (ET) is currently the only method that allows direct three-dimensional visualization of macromolecules *in situ*. Although the technique has the potential to reach a resolution of 2-3 nm, the highest resolution reported to date is only 4 nm. The main factor limiting the resolution is the low signal-to-noise ratio (S/N) that results from electron radiation damage to biological material. Increasing the electron dose that specimens can tolerate would be the simplest way to improve the S/N. Most of the previous reports used liquid nitrogen as cryogen, and the total electron dose used is around 100 e/Å². In electron crystallography, it has been recognized that cooling the specimen to liquid helium temperature provides a significant improvement in the resistance to radiation damage. Therefore, it is expected that liquid helium cooling would be advantageous for ET as well. However, the optimal electron dose at liquid helium temperature or the optimal temperature for ET has not been examined. Therefore, we analyzed electron diffraction data from thin 3-D crystals of F41, a core fragment of flagellin from *Salmonella* and 2-D crystals of bacteriorhodopsin (bR) and quantitatively evaluated radiation damage under different conditions: at accelerating voltages of 300 kV and 200 kV, at a few different temperatures, and for specimens frozen in different solutions. The measure for radiation damage is the reduction of diffraction intensities from protein crystals. We will report optimal conditions for high-resolution ET.

1P055 多種の処理ツールの統合による半自動3次元再構成システム
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Development of Three-Dimensional Reconstruction System by integration of many processing tools
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The steps for reconstructing the three-dimensional density of protein from two dimensional projection images from electron micrographs by computational methods are very complicated as well as require many image process. We have ever developed a new integration system, Semi-Automatic Three-Dimensional Reconstruction System (SA-3DRS) using "makefile", for improving time and learning efficiency for reference-based 3D reconstruction and refinement.To test the availability of the system, we applied to test images from atomic coordinates of cytochrome c oxidase and two sets of real electron microscopic images (netatively-stained apoferritin taken as tilt series & frozen-hydrated GroEL). We compared it with that on manual, and, in addition, checked the usefulness of parallel processing using "make".We could obtain a 3DR image by one step using initial projection angles of each particle, as a result of the test image and the apoferritin images with tilt series. Furthermore, by refinement process of projection angles using the initial 3DR and 2D apoferritin images, we succeeded to obtain the 3DR image with better correlation values with electron microscope images than the initial 3DR. After the initial 3DR image was in success obtained using an atomic coordinates of GroEL, we are now challenging the refinement of GroEL images obtained from electron cryo-microscope, and will report the progress in the meeting.

1P057 固体NMRによる完全水和マルチラメラベシクル中の脂質分子の局所運動性解析
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Determination of Local Mobility of Lipid in Fully Hydrated MLV by Solid State NMR
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We have developed a separated amplified local field NMR spectroscopy under magic angle spinning (MAS) which enables to determine motionally averaged heteronuclear dipolar interaction without expensing long experimental time as in normal 2D-NMR schemes. The local mobility of POPC molecules in fully hydrated multi-lamella vesicles (MLVs) was examined. The heteronuclear dipolar interactions were determined after 1D FT of minimum evolution of 2D experiment obtained from above technique. The reduced peak intensities due to recoupled ¹H-¹³C heteronuclear dipolar interaction in well-resolved natural abundant ¹³C high resolution signals were monitored with evolution of dipolar recoupling time under constant time evolution. Dynamic order parameters (DOPs) for lipid molecules were thus obtained by comparing the motionally averaged ¹H-¹³C dipolar interactions with respect to the static ones. Sufficient signal reductions were observed except for the methyl carbons from the C_γ at polar head and terminal of acyl chains. For the other sites were obtained. Dynamics map for DOPs was obtained from the sites of resolved signals. Segmental mobility for biomolecules bound to lipid bilayer can be detected based on this technique.