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Antimicrobial peptides (AMPs) play important roles in the host innate defense mechanism for different organisms. Such killing of the target cells was believed to be through the interaction with the microbial membranes with a subsequent pore-forming that leads to the permeation of biomembranes. Several models have been proposed according to the membrane structure types during pore-formation: “barrel-stave”, “carpet” and “toroidal-pore”. Based on our previous study, a series of cationic α-helical peptides with 20 amino acids has been designed and synthesized, in which two of such *de novo* designed AMPs exhibited the most significant antimicrobial activity and selectivity against various Gram-positive and Gram-negative bacteria. In the current study, to distinguish the type of membrane-peptide interactions and to understand the difference in mechanism between artificial and natural AMPs, we apply DOPC/DOPG (3:1) membranes mimicking a bacterial cell membrane system to investigate the physical factors that participate in the interaction. Peptides adopted are GW-H1 and GW-Q4 (artificial), as well as melittin and pleurocidin (natural). Both the lamellae and liposomes were used as platforms for membrane. The biophysical techniques applied include oriented circular dichroism, lamellar X-ray diffraction and small-angle X-ray scattering, with which the change in thickness of membrane bilayer of small unilamellar vesicles in solution can be measured. All the physical measurements are conducted during experiments and applied as an individual function of peptide-to-lipid molar ratio (P/L). The results show that artificial antimicrobial peptide GW-H1 and GW-Q4 behave in a different manner from the natural peptides melittin and pleurocidin. It is indicated that GW-H1 and GW-Q4 adsorbed onto the biomembrane surface continuously and in parallel, instead of attaching perpendicularly in membrane *per se*. The membrane therefore becomes thinner and thinner with, however, no perpendicular peptide orientation observed. Compared with the particle size measurement from Dynamic Light Scattering, this suggests that the liposome membrane structure has not been seriously interrupted. However, previous calcein leakage experiments strongly suggested the exchange of materials through membrane. To explain such discrepancy, a concept of transient pores or temporary loss of barrier functions of the biomembrane is introduced, by taking the changes in thickness and surface tension of membrane, as well as the influence by thermal fluctuations into consideration. In contrast, the natural peptide melittin apparently inserts itself into the membrane as described for the toroidal-pore model. In addition, our results provide clear evidence for the electrostatic effects on the initial steps of cationic AMP binding to biomembranes. Thus, through our studies, we have established a very efficient and successful methodology in the membrane research regarding the helical peptide binding, which has been quite difficult to approach before.

Keywords: antimicrobial peptides, oriented circular dichroism (OCD), small-angle X-ray scattering (SAXS)

MS04.P06

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Use of an inexpensive diffractometer for acquisition of SAXS data

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Small angle x-ray scattering (*SAXS*) is widely used in structural studies of non-crystalline or quasi-crystalline materials. SAXS is a small-angle scattering (SAS) technique in which scattering by a sample with inhomogeneities in the nm-range, is recorded at low angles (typically 0.1 - 10°). This angular range contains information about the shape and size of molecules, and characteristic spacings (including pore sizes) within partially ordered materials.

Separation of the weak scattered intensity from the strong main beam is the major obstacle that must be overcome in SAXS measurements. This becomes increasingly difficult with decreases in the desired angle. Dedicated SAXS instruments are often used to overcome this problem. In principle the separation can be effected by focusing the beam. In the past this was difficult as large bent mirrors are required. Improvements in x-ray optics have lead to the development of mirrors that not only focus the beam, but also produce monochromatic x-ray. Previously we demonstrated that with a few simple modifications high quality SAXS data on materials can be acquired using a CCD area detector and focusing x-ray optics, a combination which resulted in a low angle limit of about 0.4° (approximately 200 Å) [1]. While this combination produced good data it proved to be impractical for occasional users.

Here we examine the use of an inexpensive powder diffractometer for collecting SAXS data. SAXS data collected on the inexpensive diffractometer is compared to data collected using focusing x-ray optics, and a point detector system with a well collimated incident beam.

[1] J.R. Deschamps, B. Melde, C. Spillman, J. Konnert, *American Crystallographic Association Annual Meeting* **2009,** July 25-30, Toronto, Canada.

Keywords: meso-porous, silica, SAXS

MS04.P07

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Structural changes and phase transition of sodium dodecyl sulfate micellar solution in alcohols probed by small-angle neutron scattering

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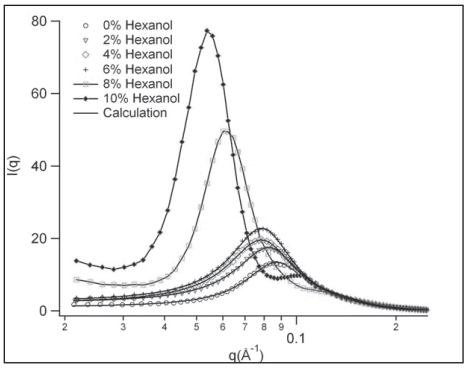
Small-angle neutron scattering (SANS) measurements on 0.3M sodium dodecyl sulfate (SDS) micellar solutions have been performed in the presence of *n*-alcohols, from ethanol to decanol at different alcohol concentrations, 2% – 10% (w/w). The ellipsoid micellar structure which occurred in the 0.3M SDS in aqueous solution with the size range of 30 – 50 Å has different behavior at various hydrocarbon chain length and concentration of alcohols. At low concentration and short chain-length of alcohols, such as ethanol, propanol, and butanol in the 0.3M SDS micellar solution the size of micelles reduced and had a spherical-like structure. The opposite effect occurred as medium to long chain alcohols, such as hexanol, octanol and decanol added into the 0.3M



SDS micellar solutions. The micelles structure changed to be more rod-like in major axis and then crossed the critical phase transition from micellar solution into liquid crystal phase as lamellar structure emerged by further addition of alcohols. The inter-lamellar distances were also depending on the hydrocarbon chain length and concentration of alcohols. While the persistent micellar structures occurred in addition of medium chain of *n*-alcohol, pentanol at all concentrations.

[1] G.M. Førland, J. Samseth, H. Høiland, K. Mortensen, *J. Colloid Interface Sci.* **1994**, *164,*163-167. [2] G.M. Førland, J. Samseth, M.I. Gjerde, H. Høiland, A.Ø. Jensen, K. Mortensen, *J. Colloid Interface Sci.* **1998**, *203*, 328-334. [3] E. Caponneti, D.C. Martino, M.A. Floriano, R. Triolo, *Langmuir* **1997***, 13,* 3277-3283.

Keywords: small-angle neutron scattering, micellar solution, micelles, liquid crystals, lamellar structure

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Structural investigation on InAs/GaSb thin films

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In the present work, InAs-GaSb super lattice thin films have been prepared and characterized. These thin films are widely used in detector technology because of their long carrier lifetimes and high detectivities. While the Molecular Beam Epitaxy (MBE) method is used for the synthesis of the studied thin films, X-ray diffraction (XRD), Dynamic X-ray simulation and X-ray scattering (SAXS and WAXS) methods have been also used to access structural knowledge. Molecular and nano scale structural information such as thickness, density, internal structure, inhomogenities, inner surfaces, repeat distances in partially ordered nano aggregations etc. have been obtained from thin film samples with surface area of 5x8 mm^2. The rocking curves related GaSb substrate (004), InAs and InAs-GaSb layers and the transmitted scattering profiles of the thin films have been recorded by using CuK_α. Fig.1. shows the XRD pattern and the simulation results of a studied sample. At the end of the structural characterizations, the well prepared samples have been determined.

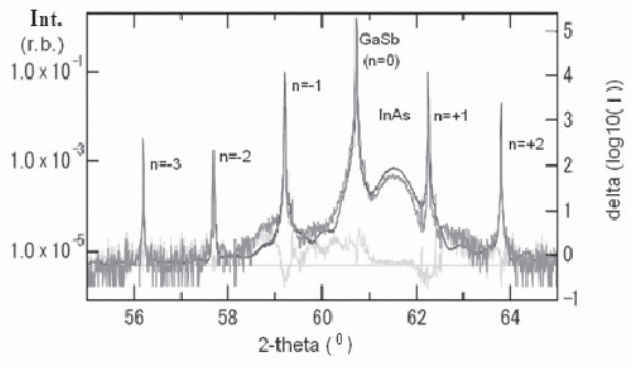

Fig.1. XRD pattern (red color) and dynamic simulation result (blue color) of a studied InAs-GaSb thin film

Keywords: thin films, InAs/GaSb, XRD, SAXS

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Examination of structural changes in the tendons during the healing process

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Tendons are bands of dense connective tissues which connect muscles to skeletal elements and transmit force generated by muscles to bones. Structurally, tendon is composed of tenoblasts and tenocytes lying longitudinally in a network of different collagen molecules. Tenocytes are responsible for the production of extracellular components of tendon that consists of collagen type I, III, V, proteoglycans, fibronectin and elastic fibrils. The largest component of tendon tissue is primarily collagen type I (COLI) and III (COLIII) which are providing unique tensile strength properties. Cross-linking between Type V collagen (COLV) and fibrils improves the forming a core structure for type I fibrils to bind and form a more stable/compact fibril package.

In the experimental researches, adult male Wistar albino rats (8-10 weeks old) were used. The reconstruction processes with/without application of tendon grafts were examined after the main phases of the acellularization of flexor tendons, reseeding of acellularized tendons *in-vitro*, *in-vivo* implantation of reseeded tendon constructs. The sutured Achilles tendons were isolated, and their 0.2-cm-long sections were used in structural analysis and mechanical tensile testing.

Before and after the mechanical testing, the structural analyses of the tendons were carried out by SAXS and WAXS methods. Molecular and nanosized structural details tried to investigate by the scattering data analysis and the constructed structural models. Structural parameters were refined by fitting experimental data with theoretical results.

At the end of the data evaluation, the present researches have showed that the native tendons may be used in improving biomaterials for tissue engineering.

Keywords: SAXS, WAXS, collagen

MS05.P01

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***In situ* diffraction studies into the formation of jarosites**

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Jarosites, $AFe_3(SO_4)_2(OH)_6$ (where A is typically K, Na or H_3O), and related minerals are of great importance to a range of mineral processing and research applications. They are deliberately precipitated in order to remove unwanted iron from process solutions in hydrometallurgical circuits. They also form in bioleaching systems and flotation circuits involving bacterial conditioning, but here they form kinetic barriers to further reaction. They occur in acid mine drainage environments and there has been a recent resurgence in interest in jarosite since its identification on Mars by the MER rover Opportunity. Jarosites are also of considerable theoretical interest as model compounds for spin frustration in kagomé-Heisenberg antiferromagnetic materials. Knowledge of their nucleation and crystallisation mechanisms is an indispensable prerequisite for the understanding of conditions which enhance or inhibit their formation thus allowing control of their occurrence in a range of environments.