on the structural features of lignin obtained from straw and bagasse sugarcane were studied using synchrotron small angle X-ray scattering (SAXS). Bagasse and straw were pretreated under three different types of pretretament -hidrothermal, diluted acid and steam explosion. The delignification was carried out by means of either soda pulping or soda/antraquinone processes. Our SAXS study was performed for aqueous solutions containing 5 mg/mL of lignin using the SAXS1 beamline of the Synchrotron Light Laboratory (LNLS), Campinas, Brazil. Data treatment was carried out by using Beaucage model for two structural levels [3].

SAXS results revealed that dilute solutions of both lignins, from bagasse and from straw, are composed of a mixture of colloidal nanoparticles and aggregates. It was observed that the aggregates in solutions of lignins from straw are in general larger than those of lignin from bagasse. The nature of the assymptotic behavior of SAXS curves at high angles allowed us to conclude that, under similar pretreatment and delignification processes, lignin aggregates from straw exhibits a fractal external surface while aggregates of lignin from bagasse shows a mass fractal structure. Our SAXS results also indicated that the diluted acid pretretament promotes a higher fragmentation of the aggregates of lignin from bagasse.

Lignins obtained from steam explosion pretreatment under different conditions of temperature do not exhibit significant changes in the fragmentation effect on aggregates and colloidal particles. The main difference regards the nature of the fractal structure, the aggregates corresponding to lignin pretreated under severe steam explosion exhibiting a fractal surface while those of lignin pretreated under softer conditions a mass fractal structure. SAXS results also indicated that delignification by means of the soda/antraquinone process promotes a lower fragmentation of the aggregates than the process of soda delignification.

Industrial applications as dispersing agent in textile segment or wastewater treatment require the use of highly fragmented lignin. Our SAXS results suggest that lignin produced by acid diluted pretreatment followed by soda pulping delignification would promote a higher yield in industrial processes.

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Keywords: characterization, lignin, SAXS

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GISAXS with nanoparticles on liquids and with multilayer films on a lab source

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The method of small angle x-ray scattering enables the investigation of materials in the nanometer scale. It is used for mesoscopic structures like colloids, partially crystalline polymers and other soft-matter samples. For a long time SAXS was mainly developed and used at synchrotrons due to the lack of high brilliance lab-sources. With the introduction of microfocus X-ray sources with high flux densities and low divergence many of useful experiments are now also feasible in the lab-environment, even GISAXS (grazing-incidence SAXS).

In this contribution we show several SAXS measurements with our high brilliance microfocus source IμS for Cu radiation. The beam was collimated with a divergence of only 1mrad and a size of about 0.5mm. The IμS was compared with conventional sealed tubes by measuring standard samples like silver behenate. Multilayer structures of thin films, which were manufactured with different techniques like e-beam evaporation and magnetron sputtering, were investigated with GISAXS in the home-lab and for a comparison at a dedicated synchrotron beamline. Nanoparticles on a liquid sample were investigated with a special GISAXS setup with an IμS and a Pilatus pixel detector. Ordering phenomena could be observed in-situ during an increase of surface pressure. The particles were transformed from single islands to an almost vertically ordered structure of connecting particles.

Keywords: multilayer, SAXS, nanoparticles

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SAXS and SANS for the better understanding of polymer processing.

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The deeper understanding of the deformation and crystallization behavior of polymer under flow is needed for the better polymer design in industries and we have focused on the researches about polymer deformation. In this talk, we will mainly discuss 'shish-kebab', a highly oriented crystal structure having an excellent mechanical property. We have clarified the role of each molecular weight component of polymer on the formation of shish-kebab structure. Previously, it was believed that the shish is mainly formed by long chains, which is necessary for the effective shish-kebab formation. However, through SANS measurement, it was found that the long chains are not the main component of shish itself and the role of long chains is to recruit surrounding chains into shish [1]. Furthermore, we have found the novel methodology for the effective shish-kebab formation using not long chains but the interaction between inorganic particles. By synchrotron SAXS and WAXD, we observed the shish-kebab formation behavior of polymers copolymerized with inorganic particles during melt drawing and clarified that the shish-kebab formation can be accelerated by controlling the degree of interaction between particles.

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Keywords: polymer, SAXS, SANS

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More possibilities of membrane permeation for antimicrobial peptides investigated with biophysical methods

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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)

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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.

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Keywords: meso-porous, silica, SAXS

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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