MS14.02.07 STRUCTURE OF POLYMER-LIKE MICELLES: SANS AND MONTE CARLO SIMULATION STUDIES. J.S. Pedersen, G. Jerke*, M. Laso*, and P. Schurtenberger*, Department of Solid State Physics, Risoe National Laboratory, DK-4000 Roskilde, Denmark; *Institut fuer Polymere, ETH Zuerich, CH8092 Zuerich, Switzerland

Giant worm-like micelles behave essentially as semi-flexible polymers in a good solvent. This is most clearly reflected in the results of scattering experiments. The scattering function shows all the features of classical polymers. Depending on the scattering vector region, one can extract information on overall size, flexibility and the cylindrical cross-section structure. However, as the micelles are self-assembling equilibrium structures, they have a large size polydispersity. The systems studied in the present work is lecithin in deuterated isooctane or cyclohexane with trace amounts of water. Detailed information on cross-section structure of the micelles has been obtained by SANS and contrast variation using heavy water. The structure was determined model-independently using the indirect Fourier transformation and square-root deconvolution techniques. In order to perform an accurate modeling of the scattering data in the full range of scattering vectors, we have performed and extensive Monte Carlo simulation study of a Kratky-Porod-type model for semi-flexible polymer chains with excluded volume effects. The scattering functions were determined and parameterized, so that they can be used for fitting the data. The fitting of the experimental data provides information on the size distribution and persistence length. The latter describes the local flexibility of the micelles. For the isooctane system the persistence length shows a pronounced concentration dependence with a value of 150 A in the dilute limit. The concentration dependence reflects the inter-micellar interaction effects in the semi-dilute regime. Our recent Monte Carlo simulations on many chain systems confirm this conclusion.

MS14.02.08 ANTIMICROBIAL PEPTIDES IN MODEL MEMBRANES STUDIED BY IN-PLANE NEUTRON SCATTERING. D.L. Worcester*, Ke He, S.J. Ludtke, W.T. Heller, T. Harroun and H. W Huang, Rice University, Houston, TX 77251-1892 and *University of Missouri, Columbia, MO 65211.

Antimicrobial peptides isolated from the host defense systems of organisms have been shown to exert their activity directly on cell membranes, but the antimicrobial mechanisms have not been elucidated, partly because the large quaternary structures formed by these peptides in membranes are difficult to establish. Many of these peptides insert into the membrane as transmembrane alpha helices when their concentrations exceed a lipid-dependent critical value. Organization of many of these peptide helices together with membrane lipid into special structures is probably a key aspect of antimicrobial action. We are using neutron in-plane scattering to elucidate these structures for several antimicrobial peptides. Using this technique we show that inserted alamethicin creates aqueous pores in membranes. Neutron data were collected for alamethicin in DLPC, deuterated DLPC and DPhPC with D2O or H2O. Alamethicin appears to form pores in the barrel-stave fashion. Calculated form factors for the pores with different deuteration conditions multiplied by a simulated structure factor, were used to fit the in-plane neutron scattering data and establish pore size as well as number density. Essentially all of the inserted alamethicin was found to be in the form of pores. Other antimicrobial peptides have also been measured with this in-plane neutron scattering technique. Results for magainin show very detailed, temperature dependent, in-plane scattering. Structures other than pores of the barrel-stave type may be present for some of the peptides.

PS14.02.09 MSANS STUDIES OF AN ANISOTROPICAL-LY-SCATTERING MICROSTRUCTURE. A.J. Allen[1], J. Ilavsky[1,2] and G.G. Long[1], [1]Materials Science and Engineering Lab., NIST, Gaithersburg, MD, [2]Plasma Spray Lab., State University of New York, Stony Brook, NY.

Multiple-SANS (MSANS) methods, recently modified to study anisotropicallyscattering microstructures, have been applied to the quantitative characterization of the coarse and concentrated pore/splat morphologies within ceramic plasma-sprayed deposits. The new MSANS formulation has been used to interpret the multiple scattering arising from the different coexisting anisotropic orientation distributions of coarse interlamellar voids and intralamellar cracks. For oblate- or prolate-shaped scatterers, this formulation considers both diffraction and refraction effects in predicting the MSANS broadening as a function of neutron wavelength. In ceramic materials, pores or voids with mean diameters of up to about 4 micrometers have proved measurable. For plasma-sprayed deposits, the MSANS studies have been combined with porosimetry and anisotropic Porod scattering measurements in a quantitative characterization of the undisturbed statistically-representative microstructures, as a function of the processing parameters or service degradation conditions. Similar MSANS methods are now being employed in the study of anisotropic crack propagation during the controlled-texture sintering of ceramic materials.

PS14.02.10 DNA AND PLPC CONCENTRATED SOLUTIONS: A SAXS STUDY OF INTERACTING SYSTEMS. L. Q. Amaral, V. Castelletto and R Itri, Instituto de Fisica, Universidade de Sao Paulo, Caixa Postal 66318, 05389-970-Sao Paulo, SP, Brazil

Results obtained by small angle X-Ray scattering (SAXS) in systems with interactions are presented, with emphasis on information obtained from both the particle form factor P(q) and interference function S(q). DNA fragments in water represent a solution of rod particles with cylindrical symmeny while PLPC (palmitoyl lisophosphatidil choline) in water form spheroidal micelles. DNA solutions are studied[1] in the isotropic (I) phase in the semidilute regime until the I-cholesteric phase transition. The interference peak position q_m as a function of concentration fits an universal curve with exponent 1/2 for an effective rod length L=340Å. The form factor of the DNA fragments is obtained from the less concentrated solution, where interference effects are not present in the measured range, and it is in good agreement with the B form of DNA. The interference curves for the more concentrated solutions are experimentally derived by dividing the corrected SAXS curve by the, particle form factor. The Indirect Transformation Method in Reciprocal Space is used to get the desmeared SAXS curve. Modeling of the interference peaks with Gaussian functions compares well with recent theories for interparticle interactions on solutions of rodlike polyelectrolytes. The peak broadening β expressed as βL in function of concentration also fits universal curve with exponent 1/2. The fitting shows that the short-range order for rods in the semidilute region has correlation length slightly above first neighbors. In the case of inhomogeneous globullar micelles as PLPC it is also possible to obtain[2] the particle distance distribution function p(r) for lower concentrations. For higher concentrations the SAXS curve is fitted to the smeared product P(q)S(q), with S(q) calculated in the mean spherical approximation. The lipid system PLPC/water is an example of isotropic solution leading to a cubic phase. Analysis of SAXS in terms of P(q) and S(q) show that the micelle form remains stable and with small anisotropy. This is in contrast with detergent/water systems, where there is micellar growth and the isotropic solution leads to an hexagonal phase.[3]

1- V. Castelletto,R. Itri and L.Q.Amaral, Macromolecules 28, 8395 (1995).
2- R. Itri and L.Q. Amaral, J. Applied Cryst. 27, 20 (1994).
3- R. Itri and L.Q. Amaral, Phys. Rev. E47, 2551 (1993).