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COMPLEXITY IN THE HITHERTO SIMPLE METALS

N. Ashcroft
Laboratory of Atomic & Solid Physics Cornell University, Physics Dept. Clark Hall ITHACA NY 14853-1447 USA

At normal pressures and temperatures many of the so-called simple metals (especially the alkali class) possess highly symmetric structures, often Bravais lattices, and in these stabilizing arrangements the measure of cell size greatly exceeds the measure of core space size (essentially the fourth moment of the localized charge density). The breaking of such symmetry can become, however, a physical possibility providing first that a condition governing relative core and cell sizes is met (that the ratio actually increases). Under such conditions, brought about at high and nowadays attainable pressures, these systems have been predicted to take up complex structures including those with pairing states for the ions at sufficiently high compressions. An important element in the ensuing electronic structure is the progressive interstitial localization of electrons where associated valence band-widths actually decline with further increase in density. Single-particle densities of states therefore also increase and enhances the prospect of ordering (charge-density-waves, electron-pairing and superconductivity, ...) in the initiating many-body problem. The quasi-localized valence electron states supplement the localized (and often highly polarizable) core states and together give rise to a re-appearance of fluctuating multipole terms emphasizing again the importance of the role of non-locality in the functional approach to their energetics, and hence also to their structural characteristics. Measured high density structures of the alkali metals are especially interesting because of insights gained from them on the manifestation of non-linear response in the valence electron system, and the bearing this has on the relative contributions of the (state dependent) pair- and multi-center interactions as they evolve with pressure. * Supported by the National Science Foundation

Keywords: THEORY OF CONDENSED MATTER, HIGH PRESSURE STRUCTURES, ALKALI METALS

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A SOFT MATTER RANDOM-FIELD SYSTEM: THE NEMATIC TO SMECTIC-A TRANSITION IN AN 8OCB-AEROSIL DISPERSION

P.S. Clegg[1] C. Stock[1] C.W. Garland[2] R.J. Birgeneau[1] A. Roshi[3] G.S. Iannacchione[3]
[1]University of Toronto Department of Physics 60 St George Street TORONTO ONTARIO M5S 1A7 CANADA [2]Department of Chemistry, Massachusetts Institute of Technology [3]Department of Physics, Worcester Polytechnic Institute

We present an x-ray scattering study of liquid crystal-aerosil dispersions. The measurements were carried out over the temperature range in which the pure liquid crystal (8OCB) undergoes a nematic (N) to smectic-A (SmA) transition. At this transition the liquid crystal develops a mass density wave in one dimension; the order parameter has continuous symmetry having an amplitude and a phase. The aerosils are 7nm-diameter silica spheres which hydrogen bond together to form a highly porous environment. This pins both the orientation of the 8OCB molecules and also the phase of the mass density wave. The SmA order is disrupted by the aerosils, which causes a broadening of the reflection from the density wave. The line shape is well described by modeling the effect of the aerosils as a quenched random field.

We have verified the surface area of the random environment from our small-angle scattering data. We show that, for intermediate levels of disorder, the random field strength is proportional to the surface area. These results, in conjunction with published light scattering data, suggest that it is the pinning of the phase of the density wave, which disrupts SmA order. Radzihovsky and Toner [PRB 60, 206 (1999)] made contrasting predictions.

We conclude that the continuous symmetry N to SmA transition in an 8OCB-aerosil dispersion is a novel soft matter random field system. Furthermore liquid crystal-aerosil dispersions will enable us to study the effect of quenched random disorder on a wide variety of soft matter phase diagrams.

Keywords: SMECTIC-A TRANSITION, RANDOM FIELD, AEROSIL

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NEW SHAPES IN SURFACTANT SELF-ASSEMBLY: FROM SOFT TO STIFF STRUCTURES AND FROM FINITE TO INFINITE SIZES

C. Vautrin[1] B. Demé[2] M. Dubois[1] A. Meister[1] Th. Gulik-Krzywicki[3] Th. Zemb[1]
[1]Service de Chimie Moléculaire, Centre d'Etudes de Saclay, F-91191 Gif sur Yvette Cedex FRANCE [2]Institut Laue-Langevin, BP 156, F-38042 Grenoble Cedex [3]Centre de Génétique Moléculaire, CNRS, F-91190 Gif sur Yvette

Lipids and surfactants form bilayers that can fold to form vesicles, ordered membrane stacks or random bilayers. A new type of self-assembled bilayer organization has been observed recently: hollow aggregates of regular icosahedral shape formed at certain compositions in mixtures of anionic and cationic surfactants (catanionics). The aggregates are stabilized by pores located at the vertices. In this ternary phase diagram, another new structure has been found: rigid nanodiscs of molecular thickness and quasi-infinite in-plane dimension. Both types of aggregates are made of bilayers of alternated positive and negative charges. Their stiffness results from the regular 2D-network of opposite charges at the surface of the aggregates that induces crystallization of the chains. Excess charges are expelled from the plane of the aggregates and give rise to the curvature required locally to built the edge or the pores of the aggregate. This yields to a local concentration of charges at the edges/pores. These are not compensated by first-neighbors like in the plane of the aggregate but by counter-ions and are responsible for a local double layer and the stability in very dilute solutions. The signature of the 2D network of charges can be observed at wide angles in particular conditions of isotopic substitution. Small- and wide-angle neutron scattering experiments have been performed at the Institut Laue-Langevin, on D22 and D16, respectively. The results obtained with these new shapes of aggregates will be presented together with X-ray scattering and electron microscopy results as well as packing simulations based on energy minimization.

Keywords: NANODISCS ICOSAHEDRA CHARGED AGGREGATES

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POLYELECTROLYTE DIBLOCK COPOLYMER MICELLES STUDIED BY SANS

J.R.C. van der Maarel[1] W. Groenewegen[1] S.U. Egelhaaf[2] A. Lapp[3]
[1]Leiden University Leiden Institute of Chemistry PO Box 9502 LEIDEN 2300 RA NETHERLANDS [2]University of Edinburgh, UK [3]Laboratoire Leon Brillouin, France

With a view to describe the charge ordering and to determine the size of spherical micelles of the diblock polyelectrolyte copolymer poly(styrene-block-acrylic acid) [PS(20)-b-PA(85)], we have obtained the partial structure factors pertaining to the core (PS), corona (PA), and counterion (TMA) density correlations with small angle neutron scattering. The PS-blocks form a densely packed spherical core with a radius 4.5 nm and an aggregation number around 100; the core structure does not depend on the corona charge and/or ionic strength to a significant degree. At full corona charge and minimal screening conditions, the PA chains in the interfacial coronal layer are almost fully stretched in the radial direction away from the core. Furthermore, a comparison of the counterion involved partial structure factors with the relevant structure factors pertaining to the PA-blocks shows that the counterion distribution along the radius is very close to the one for the segments of the corona-forming blocks. With increasing salt concentration and/or lower fractional corona charge, the micelle contracts and it is shown that the corona chain statistics can be described by scaling theory for osmotic star-branched polyelectrolytes. For low degree of ionization, the charges were observed to migrate to the outer corona region (charge annealing). The dimension of the micelles and the radial scaling of the corona charge density are discussed in terms of a balance of the elastic, conformational, stretching forces and the osmotic pressure exerted by the co- and counterions trapped in the coronal layer.

Keywords: POLYELECTROLYTE COPOLYMER MICELLES