frequency of one pattern every 135 ms (25 ms of acquisition time and 110 ms of readout time). The results show a complex sequence of reactions including the formation of several intermediate phases, which then lead to the formation of a simple biphasic product of small round particles of TiC embedded in a large grained NiAl matrix. A possible synthesis mechanism has been proposed to explain the formation of this composite. In order to determine if both combustion modes lead to the same synthesis mechanisms, recent results on the same reaction studied in explosion mode using time-resolved neutron diffraction will be presented and compared with the time-resolved X-ray diffraction results.

Keywords: time-resolved diffraction, combustion synthesis, NiAl/TiC composite

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MS56 ANALYSIS COMBINING SANS AND SAXS EXPERIMENTS
Chairpersons: José Teixeira, Roberto Triolo

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Hydrophobic Polyelectrolytes: Combined Small-angle Neutron and X-ray Scattering Studies

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The structure of salt-free aqueous solutions of highly charged hydrophobic polyelectrolytes was investigated using high-resolution small-angle neutron and X-ray scattering. The choice of one technique rather than another was driven by the contrast between the solvent (H_2O and/or D_2O) and the species (macroions and/or counterions) we want to look at. Various architectures of sulfonated polystyrene macroions with distinct sulfonation rates as well as distinct counterions were considered.

We will present scattering results that show strong evidence for the existence of necklace conformations with dense charged aggregates connected by stretched chain parts. Such conformations have been predicted on the basis of scaling arguments for weakly charged polyelectrolytes under poor solvent conditions [1] and have been confirmed by low-resolution small-angle X-ray scattering studies [2] and molecular dynamics simulations [3]. They result from the balance between the tendency to precipitate, the electrostatic repulsion and the entropic degrees of freedom. It was however suggested that fluctuations should impose a severe obstacle in observing these necklace structures [4]. Here, we are more concerned with quenched polyelectrolytes and the non-sulfonated sequences may form microdomains. The resulting shape could therefore be similar, though the physical case is not the one theory was made for.

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Keywords: SANS, SAXS, hydrophobic polyelectrolytes

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Utility of Absolute Calibration in SANS and SAXS Studies of Polymers and Colloids

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Absolute calibration forms a valuable diagnostic tool for the detection of artifacts in SANS and SAXS experiments. This lecture emphasizes the importance of placing data on an absolute scale, in units of cm^{-1} and reviews the methods available to accomplish this. In order to minimize the time associated with calibration, emphasis is placed on the development of strongly scattering standards which may be run in brief time periods, and special attention is paid to those that can be used for both neutron or X-ray experiments. Independent calibrations of such standards may be tested by comparison with the theoretical relationship between the x-ray and neutron cross sections.

The use of absolute units is not essential for measuring the spatial dimensions, though the cross section is a sensitive indicator of whether an appropriate structural model has been chosen. Thus, scattering from colloidal micellar solutions may be modeled by core-shell structures as a function of a set of parameters such as the inner/outer radius etc. On an arbitrary scale, it is possible to produce excellent fits of the *shape* of the scattering, which may be in error by *orders of magnitude* in intensity. Absolute calibration allows such artifacts to be recognized, and to restrict the model parameters to those which reproduce the observed cross section. Conversely, even an approximate (± 25%) calibration is sufficient to confirm the assumptions of the structural model chosen. The utility of absolute calibration in small angle scattering will be illustrated by examples comparing model calculations and experimental data from a range of polymeric and colloidal systems.

Keywords: X-ray scattering, polymers and colloids, neutron scattering

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The Structure of DNA+Cationic Liposome Aggregates Studied using SAXS and SANS

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DNA forms aggregates with electrostatically neutral phospholipids in the presence of metal cations or cationic surfactants. These aggregates can be used as nonviral vectors for DNA transfer and expression in cells [1, 2]. Synchrotron small-angle X-ray diffraction (SAXD) shows the formation of condensed lamellar phase L_α^c of periodicity d~7-8 nm with DNA monolayers intercalated between lipids bilayers due to interaction of DNA with unilamellar or multilamellar liposomes from saturated and monounsaturated phosphatidylcholines in the presence of divalent cations (Ca^{2+}, Mg^{2+}). Lipid bilayer thickness was determined by analyzing small-angle neutron scattering (SANS) curves of unilamellar liposomes according to three shells model, which devides the bilayer into two polar head group regions separated with nonpolar hydrocarbon region [3]. The inter-helical DNA-DNA distance d(DNA)~4-6 nm was observed in aggregates formed with multilamellar liposomes. Applying repeated heating-cooling process, reflection from DNA helices organization disapeared.

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Keywords: DNA-cationic liposome, SAXD, SANS

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The Subunit Arrangement of the Type I Restriction Modification Enzyme M.AhdI

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Type I restriction-modification (R-M) systems encode multisubunit/multidomain enzymes. Two genes (M & S) are required to form the trimeric 160kDa methyltransferase that methylates a specific base within the recognition sequence and protects DNA from cleavage by the endonuclease. SAXS revealed an unusually large structural change in the methyltransferase following DNA binding; this involves a major repositioning of the subunits of the enzyme, resulting in a 60Å reduction in the dimensions of the enzyme on forming a complex with DNA.

The type I R-M enzyme M.AhdI has been prepared in two