



**Experiment title:**

High pressure SAXS study of the interaction between nanoparticles

**Experiment number:**

SC 3851

<b>Beamline:</b> ID02	<b>Date of experiment:</b> from: 03/10/14 to: 06/10/14	<b>Date of report:</b> 05/03/15
<b>Shifts:</b> 9	<b>Local contact(s):</b> Dr. Johannes Möller	<i>Received at ESRF:</i>

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**Report:**

The purpose of the performed experiment was the determination of the pressure dependence of the particle–particle interaction potential of well defined dense nanoparticle systems. In our previous studies on concentrated protein solutions, the particle–particle interaction was theoretically modelled by a sum of attractive and repulsive potentials, including a screened repulsive Coulomb and an attractive van der Waals potential. For dense protein solutions, a pressure dependent, nonlinear behavior of the attractive part of the interaction potential was found [1].

In the study conducted here, we set out to explore the effect of pressure on the potential constituents separately. To this end, nanoparticles were used. The interaction potential of these simple structured particles can be tuned, e.g., by a change of pH, the addition of salts or by surface modifications.

This high pressure SAXS experiment was performed at ESRF beamline ID02 using an incident energy of 16 keV with a custom-built high pressure cell. Measurements were performed at pressures between 1 and 4000 bar. The SAXS signal of concentrated nanoparticle solutions can be described as a product of the form factor,  $P(q)$ , and the effective intermolecular structure factor,  $S(q)$ , of the particles.

FIG. 1 displays a comparison between the measured form factor and a calculated form factor. For the calculation, the nanoparticles were modeled by slightly polydisperse spheres with an

average radius of 54.5 nm (see FIG. 1). For a precise calculation of the structure factor, the calculation of the form factor has still to be optimized. Further aspects will be taken into account in the ongoing data evaluation and refinement: different size distributions, even asymmetric, will be tried. The full data analysis is still in progress.

Even without knowledge of the precise form factor, one can clearly see a pressure dependent change of the scattered intensity (see FIG. 2). Changes in the scattered intensity indicate changes in the structure factor (and therefore the interparticle interaction potential), assuming a stable shape and form factor of the nanoparticles. The pressure dependent changes of the interaction potential between the nanoparticles will be compared to the results found for lysozyme [1]. In contrast to the complex scenario of interaction forces exhibited by the protein, nanoparticles are a much simpler model system due to their well-defined surface properties and their rigid inner structure. This comparison, similarities and differences, will also help us understand the interaction potential of colloidal systems, including, for the first time, also its pressure-dependence.

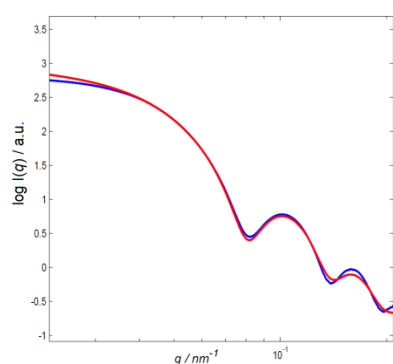


FIG. 1: Measured (blue) and calculated form factor (red). The nanoparticles were modeled by slightly polydisperse spheres with an average radius 54.5 nm.

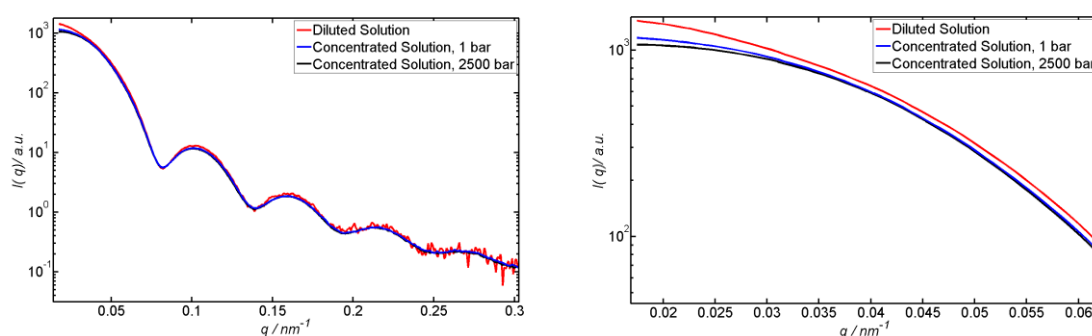


FIG. 2: Scattered intensity of a diluted nanoparticle solution (red), a concentrated solution at 1 bar (blue) and a concentrated solution at 2500 bar (black). A small but significant pressure dependence of the scattered intensity for small  $q$ -values is observable.

[1] M. A. Schroer, J. Markgraf, D. C. F. Wieland, C. J. Sahle, J. Möller, M. Paulus, M. Tolan, and R. Winter, *Phys. Rev. Lett.* 106 (2011) 178102; [2] Y. Liu, W.-R. Chen, and S.-H. Chen, *J. Chem. Phys.* 122 (2005) 044507; [3] S. Longeville, W. Doster, and G. Kali, *Chem. Phys.* 292 (2003) 413.