

FoPra SANS-1: Small-angle neutron scattering on magnetic nanoparticles

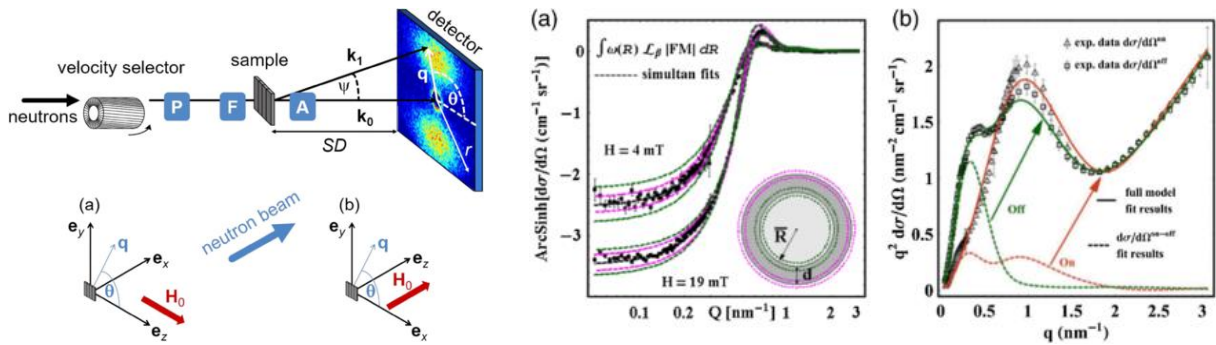


Figure 1: Left: Typical diagram of a SANS instrument, with P-polarizer, F-spin flipper, A-analyser. Below, two typical scattering geometries for magnetic SANS measurements. From [1]. Right: SANS measurement data of Co-based ferrofluid with core-shell nanoparticles. From [2].

Introduction:

Small-angle neutron scattering (SANS) can be used to investigate mesoscopic length scales and correlations from 30\AA to 3000\AA in bulk samples. The typical applications are very broad, ranging from studies of morphology and precipitate growth in metallic materials and alloys, biological structures and molecules, to magnetism on the nanoscale and fundamental questions in solid state physics. A compact summary of the applications of small-angle magnetic scattering is given in [1].

Magnetic nanoparticles are often iron, iron oxide, ferrite or cobalt based bulk particles in the range of a few nanometers to a few tens of nanometers. A suspension of these magnetic nanoparticles in a liquid medium is called a ferrofluid. The magnetic properties of ferrofluids are strongly dependent on the size and shape of the particles, ranging from superparamagnetic behaviour with small particles to ferromagnetism with increasing size. At high concentrations of nanoparticles in a ferrofluid, correlation effects also become important. The applications of magnetic nanoparticles are manifold, from magnetic hyperthermia in cancer therapy to magnetic dampers and actuators to fundamental questions in solid state physics.

The investigation of the magnetic properties of magnetic nanoparticles and ferrofluids demonstrates very well the strength of small-angle scattering with neutrons. Due to their magnetic moment, neutrons are sensitive to both the nuclear structure of the nanoparticles and their magnetic properties. A measurement using neutrons allows the shape, size and size distribution as well as the magnetization of the particles to be recorded microscopically using statistically relevant methods. In recent years, the modelling of the magnetic properties of samples at mesoscale lengths using micromagnetic theory has also made great progress.

The aim of this lab course is to work out the basics of small-angle neutron scattering and then to investigate some selected samples of magnetic nanoparticles and ferrofluids. For this purpose, a digital version ("digital twin") of the neutron small angle system SANS-1 will be used. The scattering experiments are simulated with numerical Monte-Carlo methods. The magnetic response and the expected SANS signal of simple nanoparticles are calculated using micromagnetic simulations.

Program:

1. The individual components of the beamline SANS-1 at the FRM II are presented and explained in detail with their function.
2. The technique of small-angle neutron scattering is explained using the digital twin of the SANS-1: For this purpose, the concepts of mean scattering length density, convolution of form and structure factor are introduced and the method of contrast variation is explained. The results are validated and fitted with simple Monte Carlo simulations using the program McStas [2-8].
3. The concept of small-angle magnetic neutron scattering is introduced by the different contributions to the magnetic contrast, e.g. by variation of the magnetization direction (spin misalignment scattering) or variation of the saturation magnetization. The basics and setup of small angle neutron scattering with polarized neutrons (SANS POL and POLARIS) are briefly explained.
4. Simple examples of micromagnetic simulations of magnetic nanoparticles are performed.

References:

- [1] Mühlbauer, S., Honecker, D., Périgo, É. A., Bergner, F., Disch, S., Heinemann, A., Erokhin, S., Berkov, D., Leighton, C., Eskildsen, M. R., & Michels, A. (2019). Magnetic small-angle neutron scattering. *Reviews of Modern Physics*, 91(1), 1–75. <https://doi.org/10.1103/revmodphys.91.015004>
- [2] Heinemann, A., A. Wiedenmann, and M. Kammel, The full potential of small-angle scattering with polarised neutrons for structure parameter evaluation in magnetic liquids, *Physica B (Amsterdam)* 350, E207 (2004).
- [3] K. Lefmann and K. Nielsen, *Neutron News* 10, 20, (1999).
- [4] P. Willendrup, E. Farhi and K. Lefmann, *Physica B*, 350 (2004) 735.
- [5] P. Willendrup, E. Farhi E. Knudsen, U. Filges and K. Lefmann, *Journal of Neutron Research*, vol. 17, no. 1, pp. 35-43, 2014
- [6] P. Willendrup, and K. Lefmann, *Journal of Neutron Research*, vol. 22, no. 1, pp. 1-16, 2020
- [7] P. Willendrup, and K. Lefmann, *Journal of Neutron Research*, vol. 23, no. 1, pp. 7-27, 2021
- [8] McStas Union Subsystem: M. Bertelsen Software for simulation and design of neutron scattering instrumentation, University of Copenhagen PhD Thesis, 2017