The GISANS_samp.comp file corresponds to the paper (available at https://doi.org/10.1063/1.4723634). The study involves spherical colloids arranged in an ordered manner on one side of a sapphire substrate and on the other side of a silicon substrate. In the intermediate near-surface layers, the planes of the hexagonal packing still exhibit order, but the in-plane orientation appears random for crystallites of size 1x1mm². The actual code assumes a face-centered cubic (fcc) lattice with three hexagonal layers (as shown in Fig. 1). The assumed crystallites are restricted to 6x6x6 colloids, which affects the sharpness of the Bragg peaks and is also a trade-off in terms of computational time. Moreover, there is non-zero diffuse scattering between the Bragg peaks. The in-plane orientation of the near-surface ordering can be altered by a single parameter, *phirot*.

The presence of the assumed crystallites results in a scattering pattern that is not entirely symmetrical, but it suffices for test purposes. The non-oriented mid-layer leads to isotropic scattering when using large sample apertures and yields single crystallite scattering with smaller sample apertures.

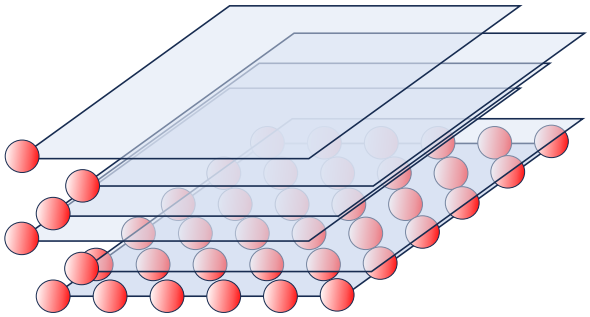

Fig. 1: The in-plane ordering of the hexagonal packing is here limited to 6x6 colloids, and there are also 6 planes in the normal direction.

The parameters of the GISANS_samp component, along with their default values, are as follows:

xwidth=0.05[m]	Dimension of the GISANS sandwich in the x-direction
yheight=0.15[m]	Dimension of the GISANS sandwich in the y-direction.
zsapph=0.02[m]	Sapphire thickness, starting from z=0 to the positive direction
zsamp=0.002[m]	Sample thickness
zsampsurf=0.000001[m]	Sample surface layer (on either side), part of the total sample
zsilicon=0.02[m]	Silicon thickness
zsiliconsurf=5e-9[m]	Silicon oxide layer thickness, part of the total silicon.
rhosapph=5.773e-6[Å^{-2}]	Sapphire scattering length density
abslensapph=163.708[cm]	Sapphire absorption length, i.e. (cross section)$^{-1}$
inclensapph=49.815[cm]	Sapphire incoherent scattering length, i.e. (cross section)$^{-1}$
rhoD2O=6.364e-6[Å^{-2}]	Heavy water….
abslenD2O=44066.347[cm]	
inclenD2O=7.258[cm]	
rhoPS=1.358e-6[Å^{-2}]	Polystyrene colloids….
abslenPS=114.502[cm]	
inclenPS=0.24588[cm]	
rhosiliconsurf=4.123e-6[Å^{-2}]	Silicon oxide....
abslensiliconsurf=401.051[cm]	

inclensiliconsurf=169.11[cm]	
rhosilicon=2.079e-6[Å^{-2}]	Silicon....
abslensilicon=209.919[cm]	
inclensilicon=9901.6[cm]	
phiPS = 0.1[vol/vol]	Volume fraction of colloids (polystyrene)
Rad = 370.0[Å]	Radius of the colloids
phirot=0.0[rad]	In-plane rotation of the near-surface crystallites
sc_aim=0.98[1]	Fraction of scattering (residual is reflected or transmitted)
sans_aim=0.98[1]	Fraction of small angle scattering vs. incoherent scattering

The neutron beam can approach the sample from any direction, whether it is in grazing incidence or in transmission SANS geometry. However, the direct entry of neutrons into the sample layers has not been fully tested yet. Currently, all scattering assumes a single scattering event using the Born approximation. Properly accounting for neutrons entering the sample directly may require multiple scattering approximations, making it more complex compared to a simple SANS transmission sample.

Within the sample component, there are additional parameters that can be adjusted, but it is advisable to do so with caution:

xidwfxy = 10.0[Å]	Debye Waller factor for crystallites in xy-plane
xidwfz = 10.0[Å]	Debye Waller factor for crystallites in z-direction
Nlz= 3	Number of different hexagonal planes (limited to 2 or 3)
Nz = 6	Total number of planes of crystallite along the z-axis
Nxy= 6	Total number of colloids in the crystallite in the x and y directions
corrlen = 3e4[Å]	Additional limit of correlation length
fudgef = 0.005	This factor is used to reduce the strong crystallite scattering to more appropriate levels, preventing excessive damping of the primary beam.

All these parameters are present in the dSigdW subroutine.

To rapidly test the GISANS_samp.comp, three instrument files are provided: GISANS_test.instr, GISANS_test2.instr, and GISANS_tt.instr. These files enable testing in both grazing incidence (impinging from front and back) and transmission geometries. It's important to note that the instrument is far from being an actual setup, but it serves as a convenient way to quickly evaluate the GISANS_samp component.

The test runs generate detector output like:

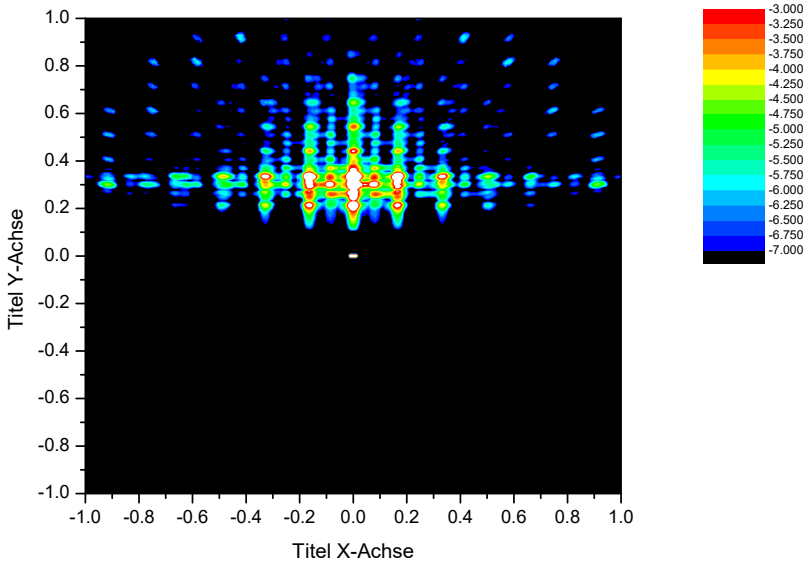

Fig. 2: The GISANS scattering is produced using the GISANS_test.instr instrument, with a logarithmic color code used to represent the data.

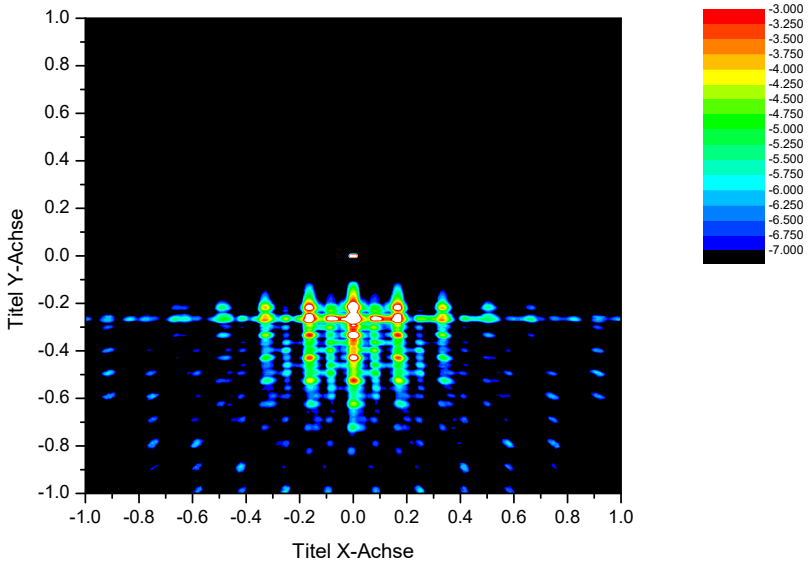

Fig. 3: The GISANS scattering is produced using the GISANS_test2.instr instrument, with a logarithmic color code used to represent the data.

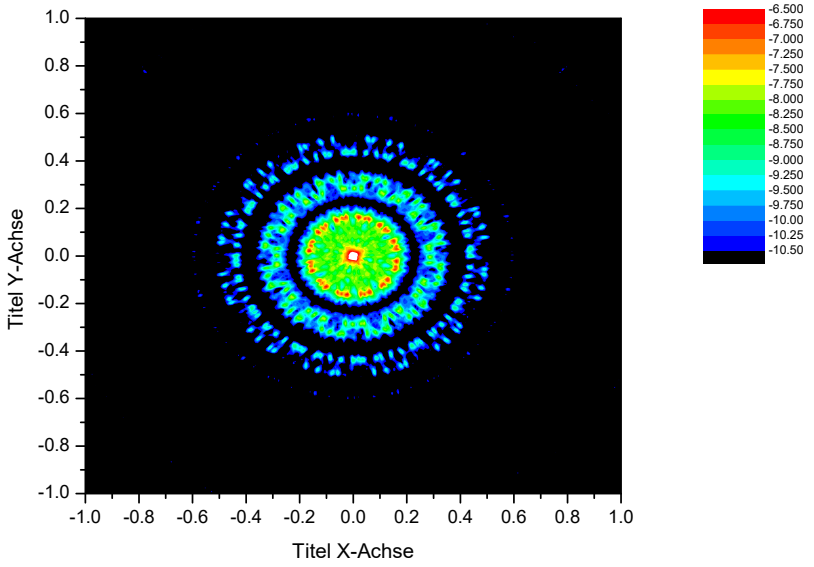

Fig. 4: The GISANS scattering is produced using the GISANS_tt.instr instrument, with a logarithmic color code used to represent the data.

The reflectometry wave field is computed using the matrix formalism initially developed by Parratt. For GISANS scattering, calculations follow the Distorted Wave Born Approximation. Notably, constructive interference between different sample layers along the z-direction is currently not considered, which is the prevailing interpretation of GISANS patterns. However, there may be exceptions to this understanding that could be explored in future implementations.

The entire GISANS_samp.comp component is still in an experimental stage. Alternative possibilities, like using hexagonally shaped crystallites instead of the current 60° parallelogram, are being considered. Additionally, there may be other potential issues that have not been fully tested yet. As a result, I welcome all critical users to offer constructive criticism.

To enhance the precision of neutron positioning at the global level, specific sub-routines were employed to control the neutron positioning, given that the latest version of MsStas appeared to generate less precise results. It's possible that there might have been an issue with the installation of McStas.

In the most recent version, the parameters have been adjusted to better match the original publication. Henceforth, we will reference this latest version for further developments:

xidwfxy = 180.0[Å]	Debye Waller factor for crystallites in xy-plane
xidwfz = 125.0[Å]	Debye Waller factor for crystallites in z-direction
Nlz= 3	Number of different hexagonal planes (limited to 2 or 3)
Nz = 6	Total number of planes of crystallite along the z-axis
Nxy= 3	Total number of colloids in the crystallite in the x and y directions
corrlen = 3e4[Å]	Additional limit of correlation length
fudgef = 0.025	A factor used to scale down the strong crystallite scattering

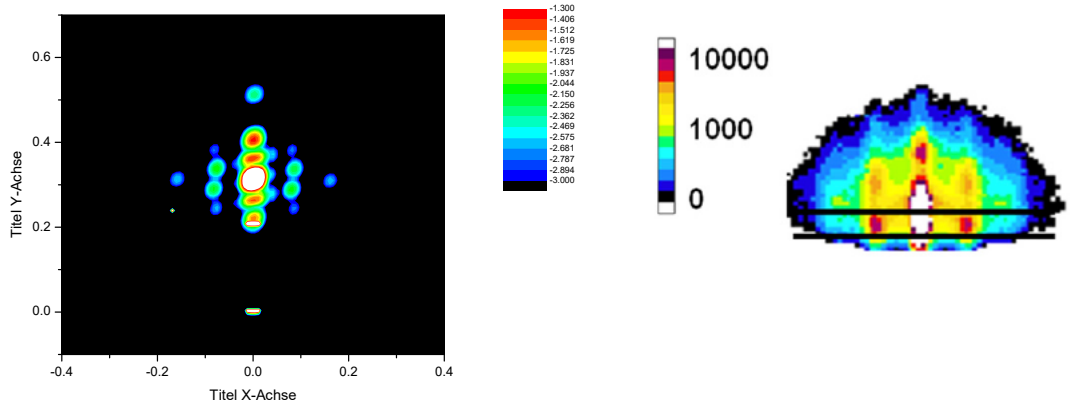

Fig. 5: The GISANS scattering is produced using the GISANS_test.instr instrument, with a logarithmic color code employed for visualization. Additionally, the original image from the publication is included for comparison.

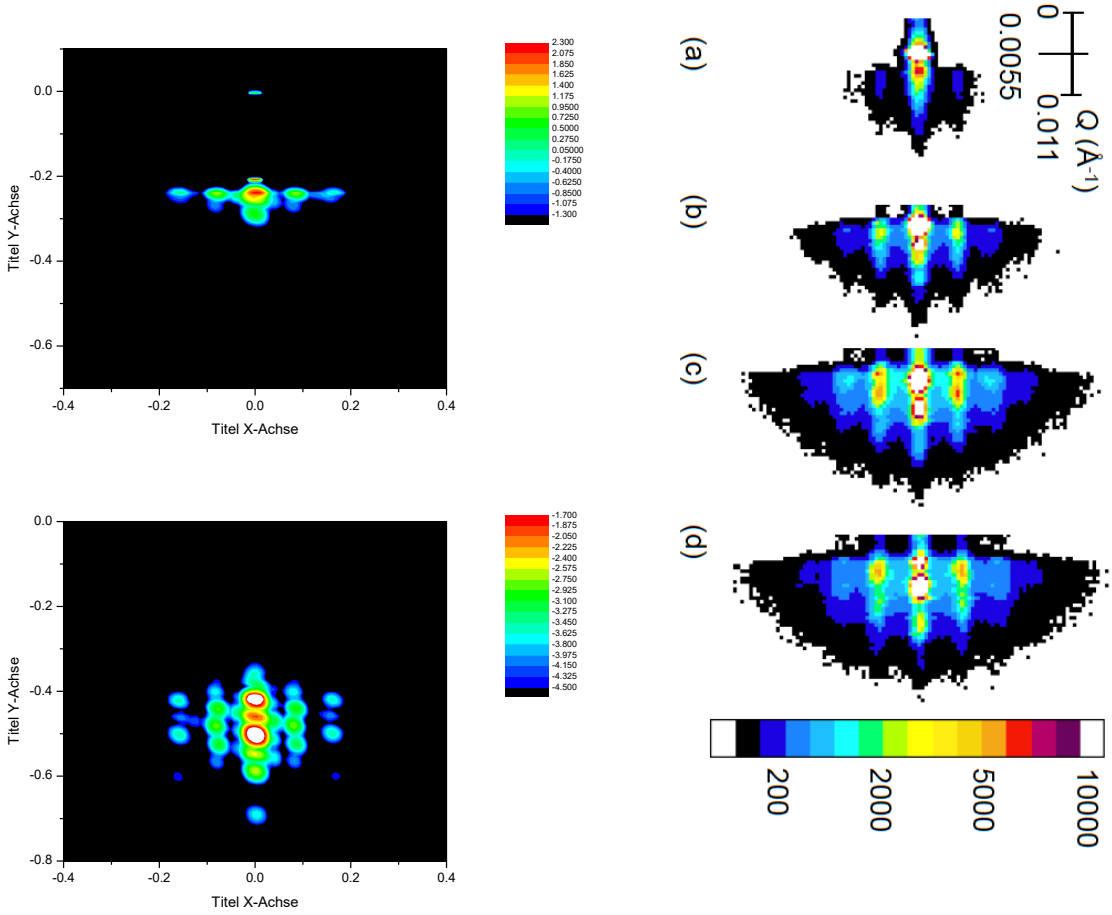

Fig. 6: The GISANS scattering is obtained using the GISANS_test2.instr instrument with incidence angles of 0.3° and 0.6°. The data representation uses a logarithmic color code. To facilitate comparison, the original image from the publication is also included.

This is also implemented in the current version of the GISANS_samp.comp component in McStas now.