SOFTWARE FOR TRANSFORMING NEUTRON SCATTERING DATA FROM INSTRUMENTAL COORDINATES INTO Q-SPACE FOR TIME-OF-FLIGHT INSTRUMENTS BASED ON IBR-2

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Essential part of polarized neutron reflectivity experiment is a conversion of neutron scattering data from instrumental coordinates into q-space. A simple approach involves cutting out the specular reflection area and then integrating with respect to the angle within the cutting out angle range. This method is actual if you need to extract only specular reflectivity, but if you want to see diffuse part of reflection it can't be used. In this case you should make a q-space map. Purpose of this work is to create software for correct transforming neutron scattering data from instrumental coordinates into reciprocal space for time-of-flight instruments based on IBR-2. The importance of this work is in the opportunity to observe and analyze not only the effects affecting specular reflection, but also the effects affecting diffuse scattering.

The program utilizes following equation [1] for converting raw instrumental data into q-space:

$$\begin{cases} q_x = \left(\frac{2\pi}{\lambda}\right)\left(cos\alpha_f cos\varphi \text{-} cos\alpha_i\right), \\ q_y = \left(\frac{2\pi}{\lambda}\right)\left(cos\alpha_f sin\varphi\right), \\ q_z = \left(\frac{2\pi}{\lambda}\right)\left(sin\alpha_f + sin\alpha_i\right), \end{cases} \tag{1}$$

where q_i – coordinates in q-space, α_i – glancing angle of incidence, α_f – polar angle of reflection, φ – azimuthal angle of reflection.

The main problem that was tackled in this work is that coordinate grid in instrumental coordinates is irregular when transformed into reciprocal space. The problem is solved by calculating density maps using custom function created in python. The software divides the q-space into pixels and counts the number of neutrons that have entered a single pixel. This program accounts for three components of q-space, it allows visualization not only of off-specular mode, but also GISANS mode.

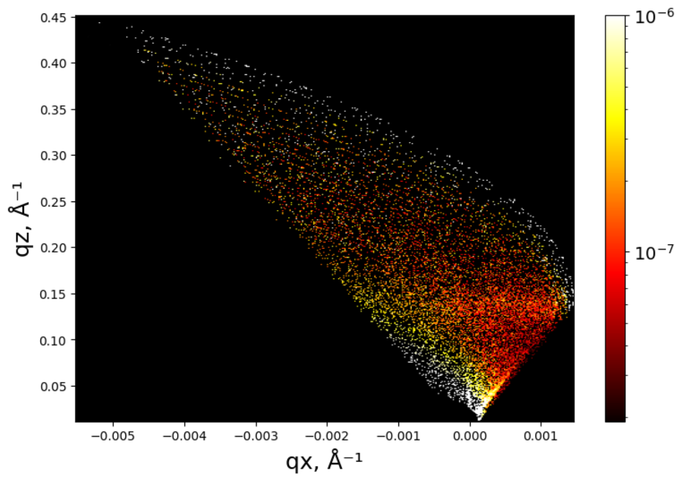

Fig. 1 – The 2D scattering map for Tb thin film

Additionally, transforming from 2D map into 1D dependence by summarizing along selected axis in q-space was implemented in program.

The software has already been used to transform neutron data obtained from scattering on the Tb thin film. This sample exhibits helicoid magnetic ordering in a narrow temperature range. Since it has a large period of approximately 4 nm, we expect that the reflection will be located at relatively small q values. However, due to the low Bragg intensity, it is difficult to detect it and determine the period of the magnetic structure using only specular reflectivity. Nevertheless, magnetic Bragg extends into diffuse scattering regions. With the latter, it is possible to detect and determine q values. 2D scattering map of Tb thin film was obtained using developed program. As Fig. 1 shows, thanks to the transformation into q-space, diffuse scattering is observed at a certain temperature, and it is possible to determine the parameters of the magnetic structure.

[1] Korolkov D. (2012). Analysis of randomly oriented structures by grazing-incidence small-angle neutron scattering. Journal of Applied Crystallography. 45, 245–254.