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*Design of neutron scattering system for the
new neutron reflectometer concept*

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1. ABSTRACT

In the field of neutron optics, neutron-scattering and neutron-reflectometry studies have yielded insight into the fundamental nature of magnetism, probed the detailed structure of proteins embedded in cell membranes, and provided a tool examining stress and strain in jet engines.

So neutrons are particularly useful in the study of materials. Thus it is important to develop the necessary techniques and systems for the proper use of neutrons in these fields. However, in order to perform neutron scattering experiments far from the reactor core where the background would be far too large to permit a proper measurement, slow and fast neutrons need to be guided to the sample and the experiment itself using neutron guides. In this sense, neutron guides act like fiber optical cable in case of light: they provide the tube from the source (the moderator) to the sample, which the neutrons with desired wavelength and energy can not penetrate so they do not escape. To accomplish this, it is very important to pay extensive attention to both the materials used for manufacturing the neutron guides, as well as the geometry of the system for a more efficient use.

We have designed and simulated a neutron instrument suit dedicated on creating a new class of reflectometers achieving high focusing and neutron flux for the given type of measurements, thus resulting in a complete and much better exploration of material structures in the field of solid state physics. This is achieved by specially designed neutron guides: in the vertical direction (perpendicular to the scattering plane) it has an elliptic shape and focuses neutrons onto the sample. In the horizontal direction it has a curved geometry in order to avoid direct line of sight, while accepting the whole beam from a spatially extended high-brilliance moderator. We have as well implemented a 5 channel multibeam illumination system using a focusing collimator. The crosstalk between the sub-beams is prevented by a set of 5 comb like slit masks and the design of the focusing collimator itself, which provide and enhance the convergence of the neutron beam.

This system will provide an exciting opportunity to design a reflectometer of the next generation to meet the increasing demand and anticipated scientific challenges.

Neutron reflectometry will assist in gaining valuable and unique information when the new neutron source and reflectometer will be developed in the near future (in the next years) and built in the far future at the Joint Institute for Nuclear Research (JINR), in Dubna, Moscow Region, Russian Federation. The anticipated research topics comprises a wide range of scientific disciplines, ranging from thin film magnetism and novel topological phases in confined geometries, over the functionality and properties of hybrid materials in the field of soft and hard matter to the structural biology of membrane proteins.

2.THEORETICAL BACKGROUND

Neutron guides

Neutron guides are used to transport beams from sources to distant locations and have greatly enhanced the ability to use neutron sources effectively by making it possible to site larger numbers of instruments far from the source where background is lower. The guides are constructed as evacuated tubes with the inner walls coated to reflect neutrons. Neutrons can only be guided into channels if they reflect off its surface at grazing angles [4]. This requires a material that could form a smooth surface with high neutron reflectivity.

For many years, neutron guides used pure natural Ni or isotope ^{58}Ni mirrors for which the limiting “critical” angle for total external reflection depends on the neutron wavelength, λ , and is $\lambda\theta_c$ where $\theta_c=0.10^\circ$ in case of Ni and $\theta_c=0.117^\circ$ in case of ^{58}Ni . Multilayer “super-mirror” coatings have been the subject of intense development work and increase the effective critical angle to $m\theta_c$ where at present m may be as large as 7. Increasing the critical angle increases the angular acceptance of neutron guides and hence the integrated transmitted intensity. However, the reflectivity of super-mirror coatings (RSM) is constant at about 99% up to $m=1$ but then falls roughly linearly with increasing m (corresponding to increasing angle of reflection) at between 6 and 10% per unit in m . This falloff in RSM has a dramatic effect on guide transmission (τ) if the number of reflections exceeds 2 or 3. Neutrons traveling through long (>30 m or so) conventional guides undergo many reflections and then super-mirror coatings give total τ little better than that for simple Ni mirrors.

So the neutron mirrors used to line the guide tubes have imperfect reflectivity and, in long conventional guides, the average number of reflections for neutron rays becomes large thus reducing the transmission. This issue is extremely important for modern neutron sources, of course it will be important for the proposed new neutron reflectometer to be constructed in the far future at JINR.

Several solutions to the problem of transporting neutrons over long distances have been proposed and currently the most favored model is that of guides with elliptic shapes. It is widely believed that elliptic guides transport neutron rays from source to sample with a single bounce, a near perfect solution for long neutron guides, and a view which is true in certain circumstances.

It is widely believed that a neutron source placed at one focal point of an elliptic guide will be imaged at the second focal point with the transported neutrons undergoing a single reflection [1]. For practical guides, which usually have rectangular cross-sections, this

becomes one bounce per dimension [2]. This one bounce transmission almost completely overcomes the problem of reduced mirror reflectivity for $m > 1$.

Some challenges in the use of elliptic guides have also been noted, e.g. that the effectiveness of elliptic guides is very sensitive to alignment. Some studies suggest that finite sources produce a coma aberration, which is basically unavoidable in real situations.

As for the geometrical considerations of neutron guides, elliptic, parabolic and curved guides are approximated by a number of constant or linear guide segments, whose ends lie on the ellipse, parabola or circle. Most of the existing neutron guides have been built this way, however there are some exceptions.

A schematic side-section view can be seen of an elliptic neutron guides and it's straight segments on the next image [2]:

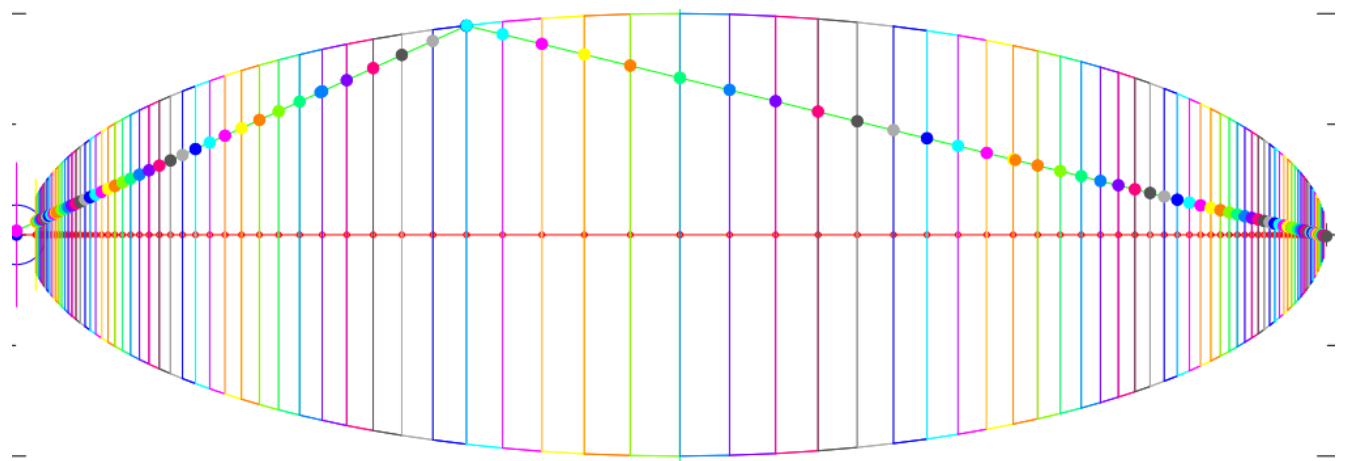


Figure 2.1: Side-section view of a elliptic neutron guide approximated by a number of straight guide segments

Neutron sources

A neutron source is any device that emits neutrons, irrespective of the mechanism used to produce the neutrons [1]. Neutron sources are used in physics, engineering, medicine, nuclear weapons, petroleum exploration, biology, chemistry, and nuclear power.

Neutron source variables include the energy of the neutrons emitted by the source, the rate of neutrons emitted by the source, the size of the source, the cost of owning and maintaining the source, and government regulations related to the source.

In the categories of sources we can distinguish between small sources, which are in general isotopes that undergo spontaneous fission and release neutrons; medium sources that are mostly plasma focusing systems and inertial confinement installations; and big sources, comprised of nuclear fission reactors, nuclear fusion reactors and high-energy accelerators (the so called spallation sources). In this last category, in the spallation sources protons that

have been accelerated to high energies hit a target material, prompting the emission of neutrons.

The IBR-2 reactor in Dubna with its unique technical approach produces one of the most intense neutron fluxes at the moderator surface among the world's reactors: $\sim 10^{16}$ n/cm²/s, with a power of 1850 MW in pulse [5].

IBR-2 is a pulsed fast reactor of periodic operation. Its main difference from other reactors consists in mechanical reactivity modulation by a movable reflector. The movable reflector is a complex mechanical system providing reliable operation of two parts, which determine the reactivity modulation: the main movable reflector and the auxiliary movable reflector. The rotors of the main and auxiliary movable reflectors rotate in opposite directions with different velocities. When both reflectors coincide near the reactor core, a power pulse is generated. It is the only reactor of this type in the world.

Nevertheless, the reactor is "ecologically friendly": it consumes very little electrical energy as compared to other research reactors, uses a very little amount of fuel (less than 20 l) which is changed once in 15-20 years.

The reactor operates continuously for a 12 day cycle followed by a shutdown to prepare for the next experiments. In addition, there is a longer shutdown to carry out necessary maintenance work during the summer time. Normally there are about 9 cycles a year.

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3. SCIENTIFIC METHODS

1. 'Virtual Instrumentation Tool for the European Spallation Source' (VITESS)

In the last years, Monte Carlo (MC) simulations have proven to be a very essential and frequently implemented tool in the optimization of existing instruments and conception of neutron scattering instrumentation for new facilities. Free open source and user friendly software packages have become available in recent years, and since then they provide an important aid for the developers of neutron instruments. In this framework the MC simulation software 'Virtual Instrumentation Tool for the European Spallation Source' has been developed

Our main working tool for designing, simulating and testing our neutron spectrometer project was the 'Virtual Instrumentation Tool for the ESS' (VITESS) software.

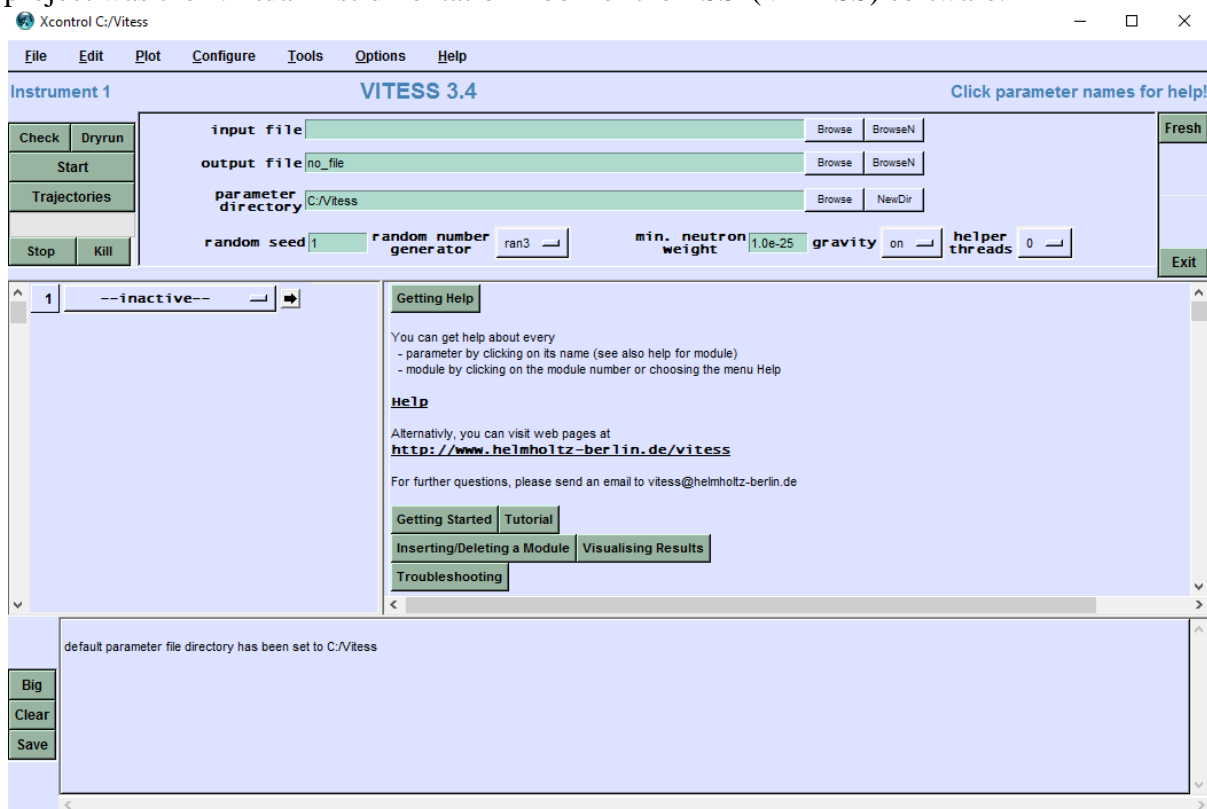


Figure 3.1: the graphic user interface of VITESS

The principle concept of VITESS is that a user can run a simulation without writing any code or using any meta-language, but advanced users can also include their own program modules. To realize that, executables controlled by parameters are used: Each component of an instrument (guide, chopper, detector, etc.) is represented by a module. Each module is delivered as an executable for the supported platforms (Windows/DOS, Unix, Linux, see above). The simulation of a component is specified by parameters and sometimes by a parameter file. These data are given to the VITESS modules via a graphical user interface.

For a whole instrument, many modules are needed. (Of course, one module may be used several times in a simulation.) During simulation, they all run independently.

The neutron beam input and output represent a number of neutron trajectories. Twelve coordinates, under the summarizing name of “vector” describe each trajectory: time, wavelength (λ), probability weight, position (x, y, z), flight direction ($\cos\alpha, \cos\beta, \cos\gamma$), spin-state (S1, S2, S3). As the 12 coordinates per neutron trajectory are consecutively written to (or read in) the user can check the changes of the neutron coordinates anywhere in the instrument and generate the statistic of the trajectories. A simulation comprises one or more modules co-working sequentially that can in principle run simultaneously. The so-called 'pipe', which is the computing core of the software works in the following manner, as illustrated in Figure 3.2:

- a. One trajectory is generated after the other, the parameters are calculated and written to the output
- b. After a number B of sets of incoming neutrons (default: B=10000, but it can be set to any desired value) are collected, the output is transferred to the next module
- c. The next module starts after the transfer

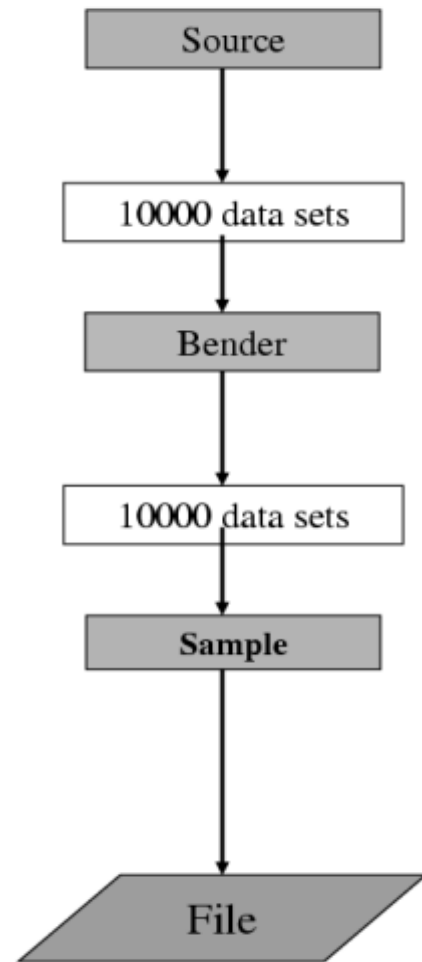


Figure 3.2: Working principle of the “pipe”

According to the presentd working principle of Monte Carlo neutron Simulations in general and of VITESS Software, every elements of virtual instrument transforms this vector, so at the exit from the set of modules the image of neutron scattering pattern can be obtained. It is imitation of real neutron transmittance of neutron beam through the set of elements of an instrument

The module '**source**' generates a neutron package of certain initial properties (position, divergence, etc.) within the ranges set by the user and propagates it to an aperture (called 'propagation window'). Now the new values are delivered to the following module that calculates the propagation of this package to its end and so on. In a mathematical sense, each package (defined by random choices) represents a random event - in VITESS it is called a trajectory. The whole set of trajectories in a simulation is the random sample. In practice each module collects typically 10000 data sets before transferring the data to the succeeding module. To avoid a need of large memories for intermediate results, the second module is started immediately after the transfer of data sets. The same holds for all other modules in the simulation.

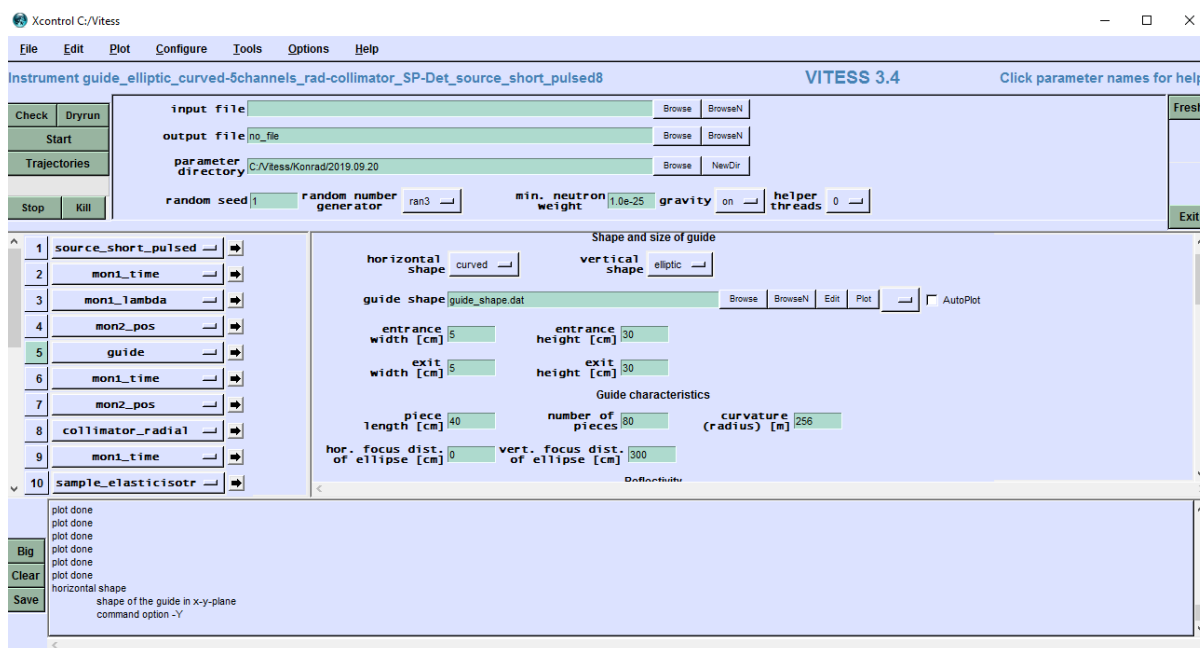


Figure 3.3: the look and parameter settings for different modules

In principle, all modules may run simultaneously in a simulation. This is the concept of piping which is suitable for DOS (Windows) and UNIX operations systems. One consequence is that a simulation can easily be split into 2 or more parts at any point of the instrument. As an example, the primary spectrometer may be simulated only once and all data sets are stored in a binary file (instead of transferring them to the following module). This file can be seen as a 'virtual source' for the second part; it is read as input to simulate the secondary spectrometer. This second part needs by far less simulation time than the first part. If the instrument variations of interest are only here, this method can save a lot of time.

For each trajectory, a count rate is calculated (depending on wavelength, number of trajectories, etc.). This count rate is diminished by reflections, absorption inside material, etc. If a trajectory does not hit a component (e.g. the sample) or the count rate is below the so-called 'minimal weight', it is removed. The sum of all trajectories gives the neutron count rate. This is calculated after each module. In this way VITESS delivers absolute count rates at each point of the instrument, which allows comparison of instruments. Flux values have to be calculated by the user himself (by dividing through the cross-section), because the true cross-section is not known to the simulation, only the upper limit, i.e. the maximal area where the neutrons can pass, not the real area.

Apart from the properties already mentioned (position, direction, and count rate), a spin-state (in 3-dimensional representation) is generated for each trajectory and the spin-orientation calculated during its flight through the instrument. Several modules exist to simulate instruments for polarized neutrons, i.e. modules for polarizers, precession fields and flippers.

Every trajectory can be identified by an ID. This allows for ray-tracing of trajectories. For all trajectories, whose ID is found in an input file, all parameters at beginning and end of each module are written to files, if the simulation is run in ray-tracing mode. Alternatively, the module 'writeout' may be used to see the whole data set, transferred from one module to

the following. In the last versions, tools were included to make the generation of input data easier or to evaluate output data.

A disadvantage of the independently running executables is that it is difficult to get (illustrative) information about the instrument as a whole.

2. Modules in VITESS

Most devices used in a neutron scattering instrument can be simulated by VITESS modules. These are basic components like source, guide, windows (or apertures), choppers, detector, several samples and numerous modules for polarized neutrons. Some of the modules can be used to simulate neutron-optical devices.

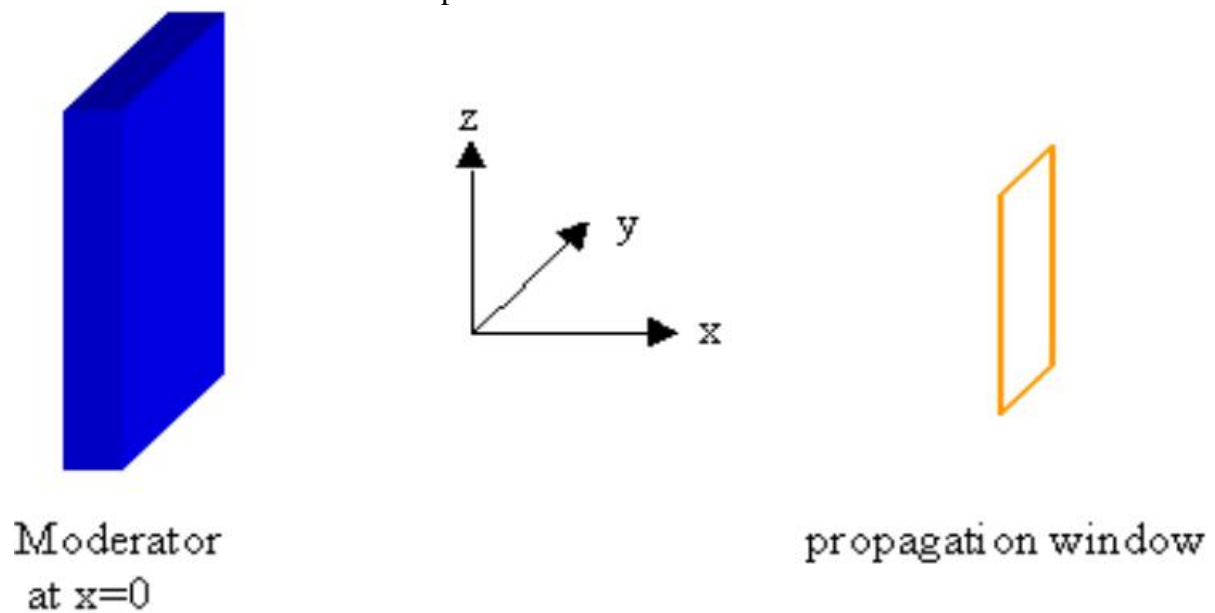


Figure 3.4: Schematic of one of the most basic module in VITESS: the neutron source, with the moderator, propagation free space and propagation window. The temperature of the moderator, neutron flux as well as other parameters have to be given too

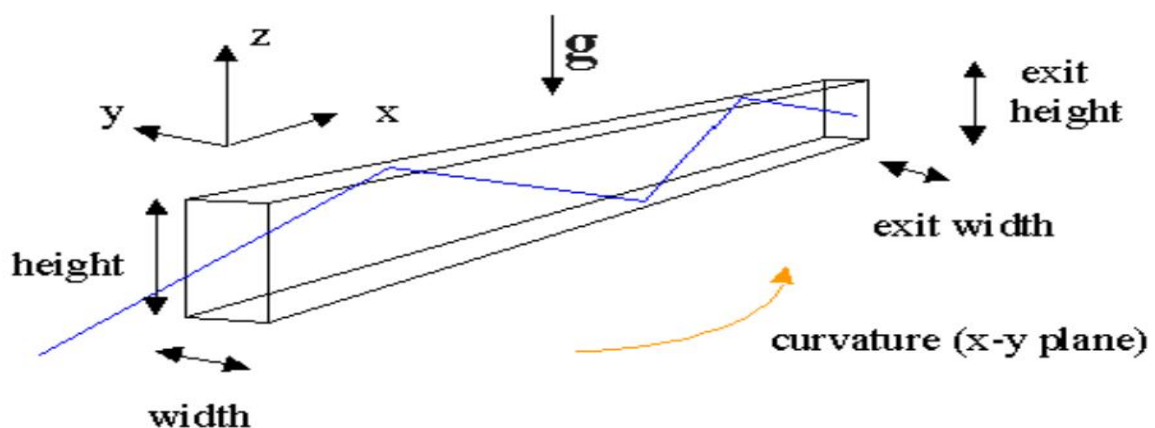


Figure 3.5: Schematic design of a neutron guide and its parameters as given in VITESS

There are several modules to monitor the intensity (= count rate) as a function of 1 or 2 parameters, i.e. as a function of wavelength, time, etc. These modules are just compressing data by binning. A range and bin size has to be given by the user. The polarization can be shown as a function of any parameter (like wavelength) by another type of monitor modules.

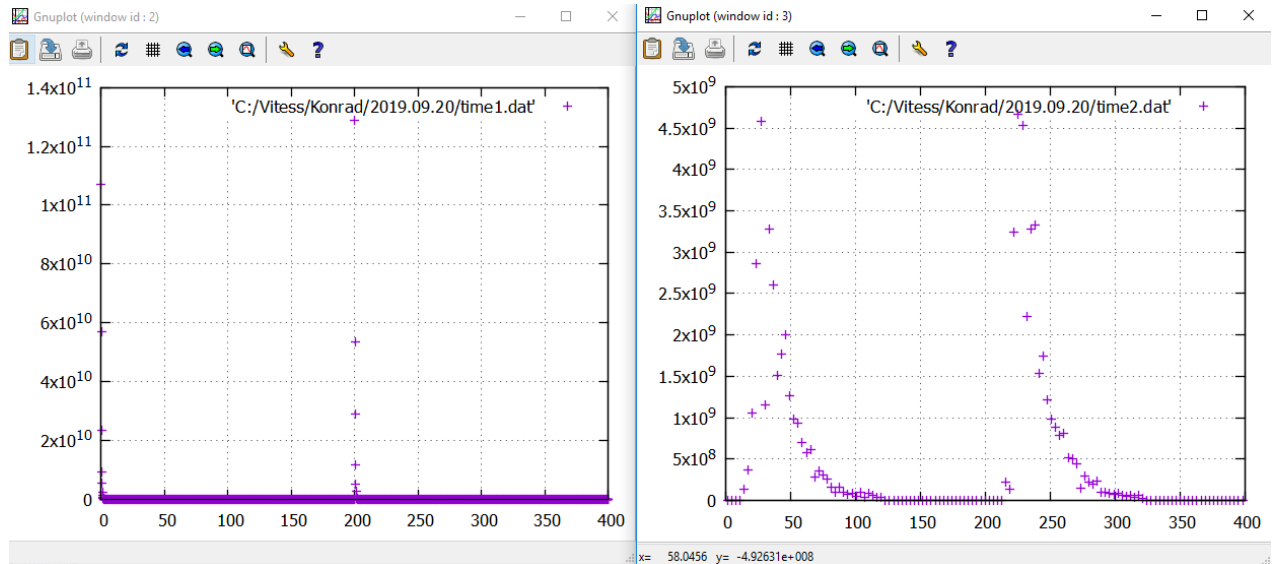


Figure 3.6: Intensity in function of time plots, as given by the embedded GNUplot in VITESS software (without any further refining or arranging of the data).

Additionally, there are two modules that do a bit of data evaluation - 'eval_elast' and 'eval_inelast'. They show intensity as a function of a parameter that is not directly used in the simulation, e.g. the d-spacing. The module 'visualize' shows the points where the trajectories hit a plane during the run (without weighting with their count rate).

The module 'writeout' writes the whole data set into a file and can be seen as a ray-tracing option. 'Frame' changes the co-ordinate system of the trajectories; any combination of mirroring, translation and rotation is possible. It can e.g. be used to realize kinks in the instrument or to simulate components that are different from the geometry assumed in the module, e.g. benders curved to the right instead of curved to the left (as realized in the bender module).

'External command' can be used by any user to integrate his own module into the simulation package. As this is not very convenient at the moment we are working on a better solution.

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4. Design and implementation of the neutron optic system. Simulation results

The aim of our research project was to design and optimize a neutron optic system for the new concept of neutron reflectometer (spectrometer) that will be developed in the near future (in the next years) and built in the far future at the Joint Institute for Nuclear Research (JINR), in Dubna, Moscow Region, Russian Federation.

Studying the literature presented in the previous chapters, we could draw some useful practical conclusions for designing our neutron optics: in case of elliptic neutron guides, the closer the focal point is to the guide entry and exit, the finer the segmentation of the guide must be (so the shorter the length piece of the guide- since the curved, elliptic and parabolic guides are usually made of constant or linear segments aligned to each other so that they form the sought form) [1;2;4].

Neutron mirrors are usually defined by their m -number, which indicates the neutron reflectance of a surface in units of reflectance ability of nickel. The critical angle for natural Ni is 0.10° and in case of the ^{58}Ni isotope it is 0.117° . So the m -number defines the $m\theta_c$ effective critical angle.

A detailed calculation of the mirror m -number at each point in the guide is important because high m -number mirrors are expensive and should be used sparingly. The source divergence and available mirror $m\lambda$ product place strong restrictions on how close the guide entry and exit can usefully be to the focal point of the ellipse.

For planning the parameters and dimensions of our neutron guide, we had to take into account the characteristics of the future neutron reflectometer and neutron source (which are not even known with 100% precision yet): the maximum wavelength band of the neutron will be from 1 Å to 15 Å; the pulse frequency is 10 Hz; the focus spot of the neutron guide has to be at least 35 meters from the moderator.

In order to avoid direct line of sight and to have a suitable geometry for the experiments, the neutron guide has to be bended in horizontal plane and elliptically or parabolically focusing in the vertical plane. Drawing inspiration from the new proposed concept of multiple channel curved guides, we have also designed our system with 5 (five) vertical channels in order to be able to realize a multibeam illumination system and to cover a much higher Q -range (the momentum difference of the neutron interacting with the sample).

One of the important criteria for our guides system was to avoid frame-overlapping: so that the slower neutrons from the earlier pulse should not coincide or arrive later than the faster neutrons from the later pulse. According to our simulation experiments, the frame of two neutron pulses is less overlapped if the dimensions of the guide are smaller (both for longitudinal as well as for lateral dimensions). For our width and height dimension range (up to 10 cm), even a guide as long as 40 meters long will not show frame over-lapping.

Frame-overlapping can also be avoided by using different kind of choppers. A neutron chopper is a rotating disk with at least one aperture. All neutrons travel the same distance to the chopper, but neutrons of different energies (and thereby different velocities) will arrive at

different times. Only neutrons of a certain velocity (energy) pass through the aperture (those that arrive when the aperture is aligned with the neutron beam), while the others are absorbed by the chopper [6]. For this reasons, this kind of choppers are called frame overlap choppers or time selectors.

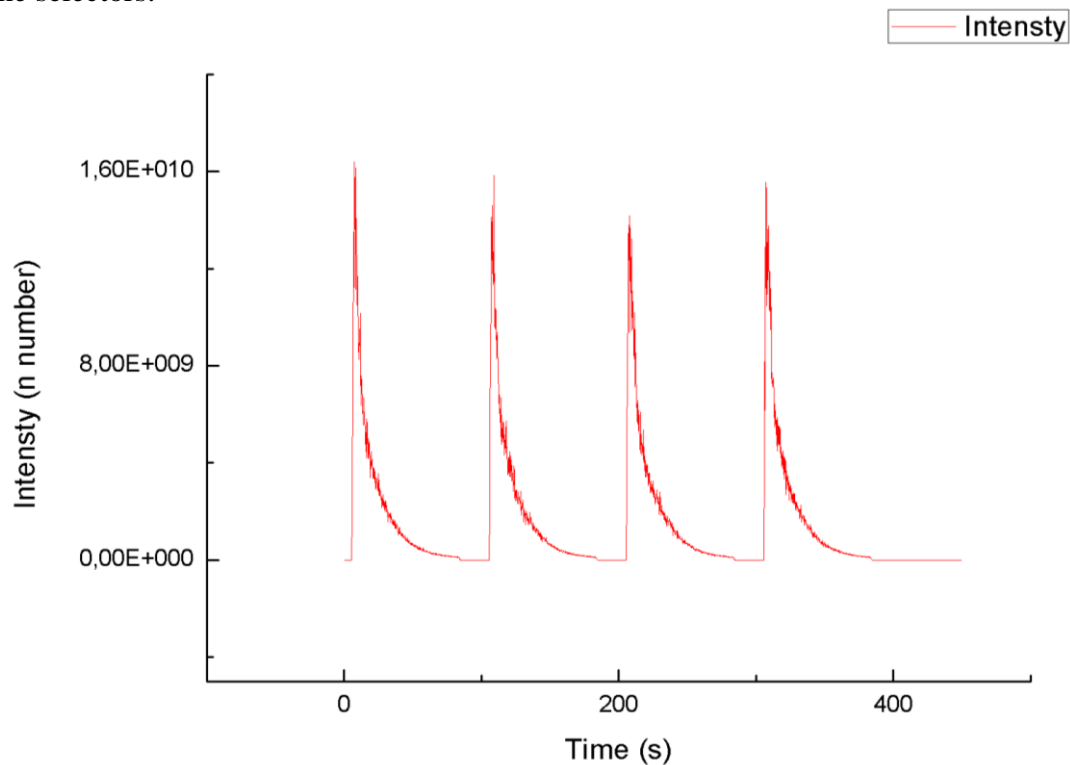


Figure 4.1: Studying frame-overlapping for the wavelength range of 0.5-15 Å, for the maximum cross-section dimensions of the neutron guide: the red plot (graph) shows the neutron intensity (count rate) in function of time after the elliptic neutron guide. Note that that the neutron pulses do not overlap in time for our range of cross section dimensions

Comparison of straight, elliptic and parabolic guides

Another aspect of our research was to find out and maximize the gain factor of elliptic/parabolic focusing guides over straight (constant) guides, as well as to compare the focusing efficiency of parabolic and elliptic designs in function of different factors. For this, we performed series of simulation experiments assessing the dependence of the gain factor on the geometric parameters of the guide. According to these, the bigger the relative height of the guide is, compared to the width, the higher the gain in neutron flux and intensity will be. So, since our height of the guide was limited (it could not be higher than 20 cm) 1 cm is the width of the guides.

The comparison of intensities for straight and focusing guides is visible in Figure 4.2. The two graphs (plots) were allegedly translated on the x axis for better illustration of the difference.

According to [4] and to other simulation experiments, the elliptic neutron guide is most efficient and suitable in case of point-like sources or spatially very confined sources of neutron (so the dimensions of the moderator has to be very low). However, in the new neutron reflectometer (spectrometer) that will be developed in the future at JINR Dubna, this

is not the case, since it will not have neither pancake moderator, neither a dimensionally confined source. Still, according to our simulations, the elliptic guide has better focusing properties than the parabolic, the two concepts being comparable (there is no order of magnitude difference between them as in case of straight v. focusing guide).

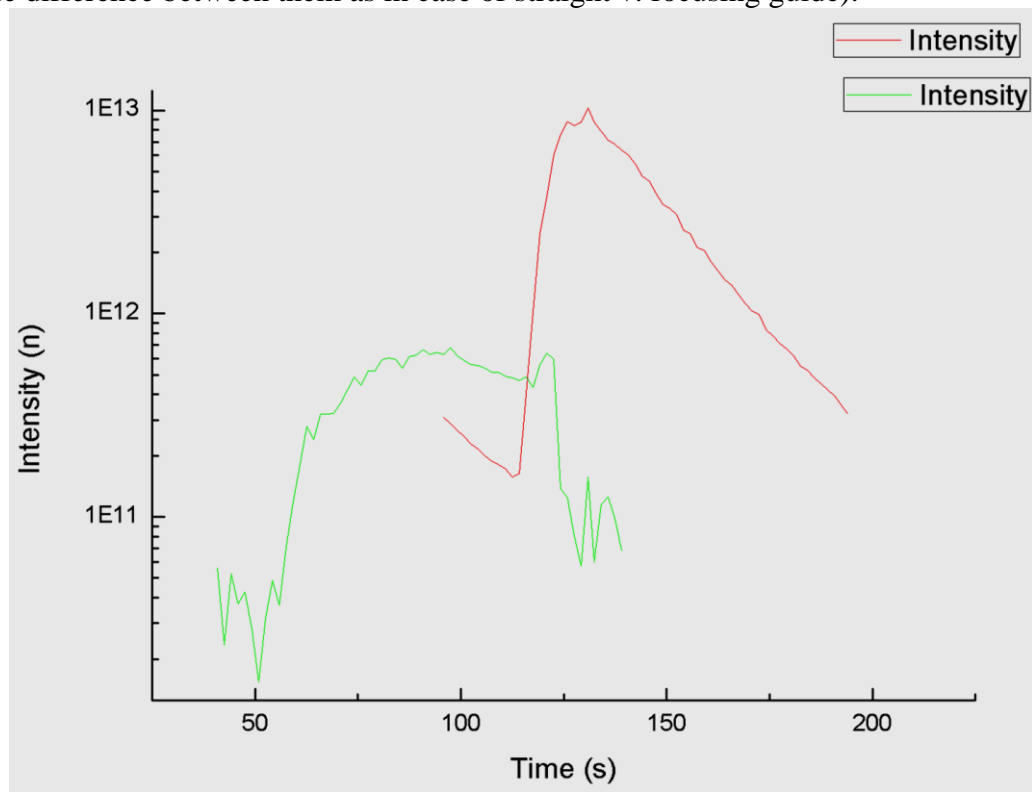


Figure 4.2: Comparison of curved focusing guide and straight guide: the red colored line represents the focusing guide while the green color is the profile for the straight guide. The gain factor for a focal distance of 4 meters in case of 32 meters long guide is approximately 12.

Another guide concept that we experimentally implemented was the double-parabolic neutron guide: in this concept, there is a parabolic guide, whose focus is behind the guide (so between the source and the guide), a straight guide segment and another parabolic guide whose focus is at the sample position (or on the detector). So this is a 3 segment symmetrical focusing system.

The idea of this system is that the focus point of the first parabolic segment is on the source (on the propagation window, which defines the divergence of the beam), whilst the last parabolic segments focus is on the sample position (or on the detector alternatively). The straight part makes the connection between the two focusing geometries.



Figure 4.3: Three segment symmetrical parabolic neutron guide system

Still, as our results show, despite the fact this design is more sophisticated and harder to realize, its focusing efficiency is still not as good as the elliptic guide's efficiency, even though they are comparable.

The most efficient guide design for the entire wavelength range from 0.5 to 15 Å is the simple parabolic guide, which is curved in horizontal direction and elliptical in vertical direction. The only difference is that the focusing property of the guide is greatly enhanced if the exit window is bigger than the entrance. Since the width of the guide has to be constant since it is bent in horizontal direction, the height is 2.5 cm higher than the 12 cm high entrance.

Below there is a comparison plot of the intensity distribution for the elliptical, trapezoid and simple straight guides for the wavelength range of 0.5-15 Å.

The next plot is a comparison of the elliptic, simple parabolic and of our special design focusing guide. Without any doubt, the simple elliptic guide with higher exit is outperforming all the other design concepts.

According to the above presented data and reasons, our neutron guide design choice will be the elliptic guide with higher exit than the entrance. Beside the much higher intensity and focus gain, this is way easier to realize from technical and engineering point of view than the complex focusing installation.

Next we had to realize the splitting of the neutron beam, between the guide and the sample, into 5 sub-beams. This work and related principles are presented in the next subchapter.

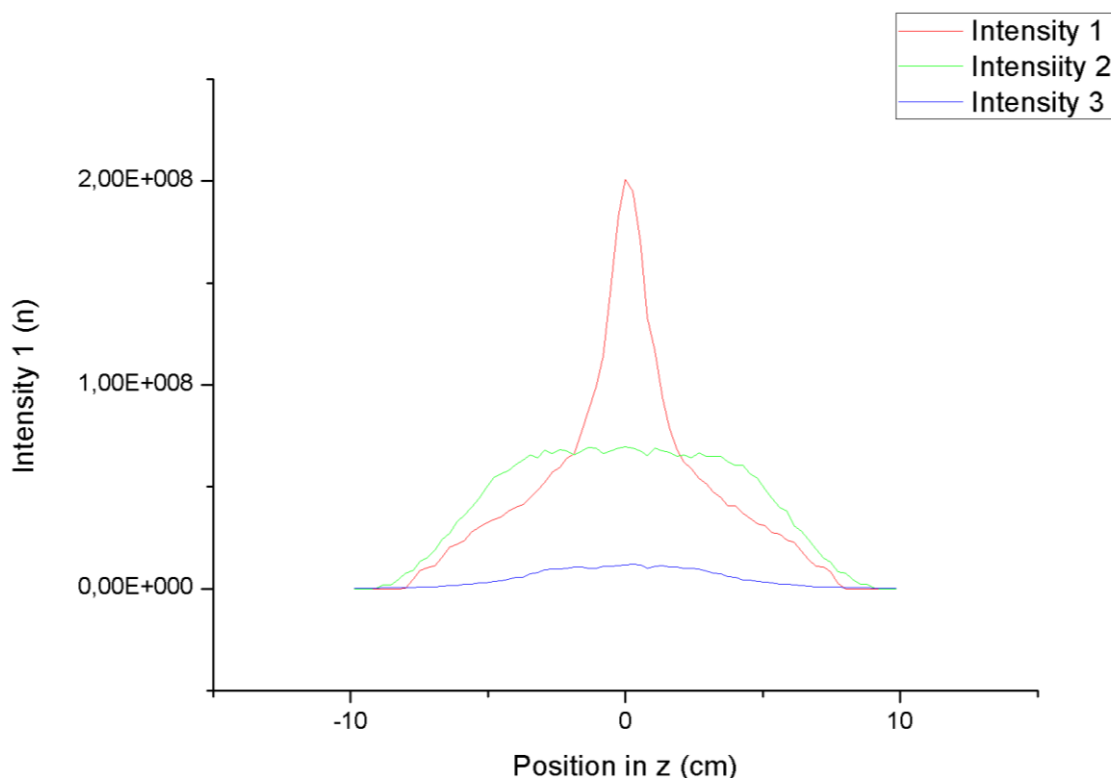


Figure 4.4: Red line is the distribution for the elliptic guide with bigger exit window than the entrance; the green one is for the trapezoid guide and the blue one is the simple straight guide

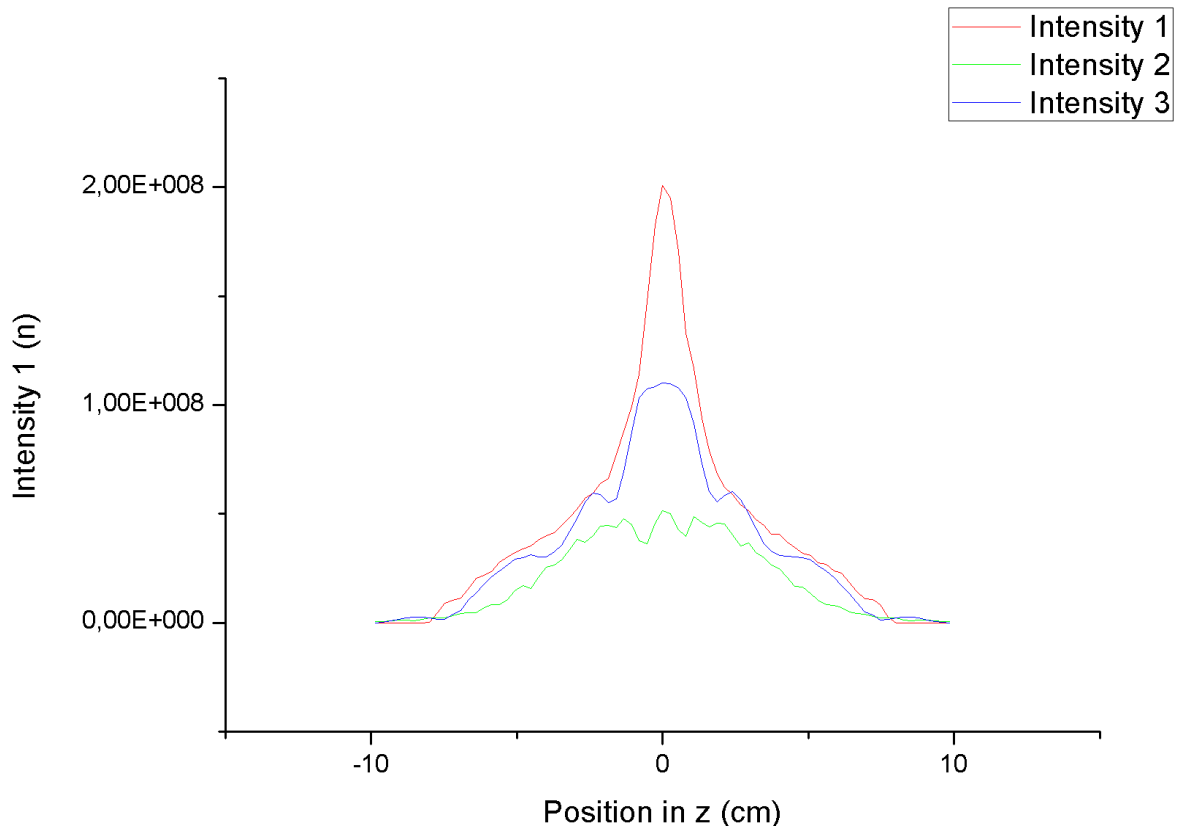


Figure 4.5: Red line is the distribution for the elliptic guide with bigger exit window than the entrance; the green one is for the parabolic guide and the blue one is our special design guide

Implementing the channel concept. Collimators.

In the Heritage reflectometer concept, the multibeam illumination system was realized with five horizontal channels in the neutron guide [1]. The spitting of the neutron beams in sub-beams is important because using this technique, we can cover a much higher Q-range (the momentum difference of the neutron interacting with the sample).

However, our design involves first of all horizontally bent and vertically focusing guide design. The channel structure and multibeam ideas were implemented using a radial collimator divided in 5 channels, rather than the guide being divided in 5 channels.

So for efficiency reasons, our idea was to implement the multibeam illumination concept using a focusing collimator at the end of the elliptic neutron guide. This way we can get a higher intensity by up to 30% compared to the case when the guide has the 5 channel structure.

Collimators reduce beam divergence for light and particle optics by geometrically defining the beam with absorbing material. For neutrons, the absorbing material is an element or compound with an isotope that has a large neutron absorption cross-section, e.g., cadmium, gadolinium, or boron.

There are two types of collimators in common use for neutron scattering instrumentation. **Soller collimators** consist of a series of thin parallel absorbing plates or septa oriented along the beam direction, and are used to define the beam divergence for linear portions of neutron instruments. The reduced divergence also improves the background from sample environment equipment. Radial collimators are usually used for the case when an instrument employs a large area of detectors to cover a wide range of scattering angles. A radial collimator consists of a series of absorbing septa radially oriented from a fixed point. Schematic images of soller collimators and a focusing collimator can be seen in the next images:

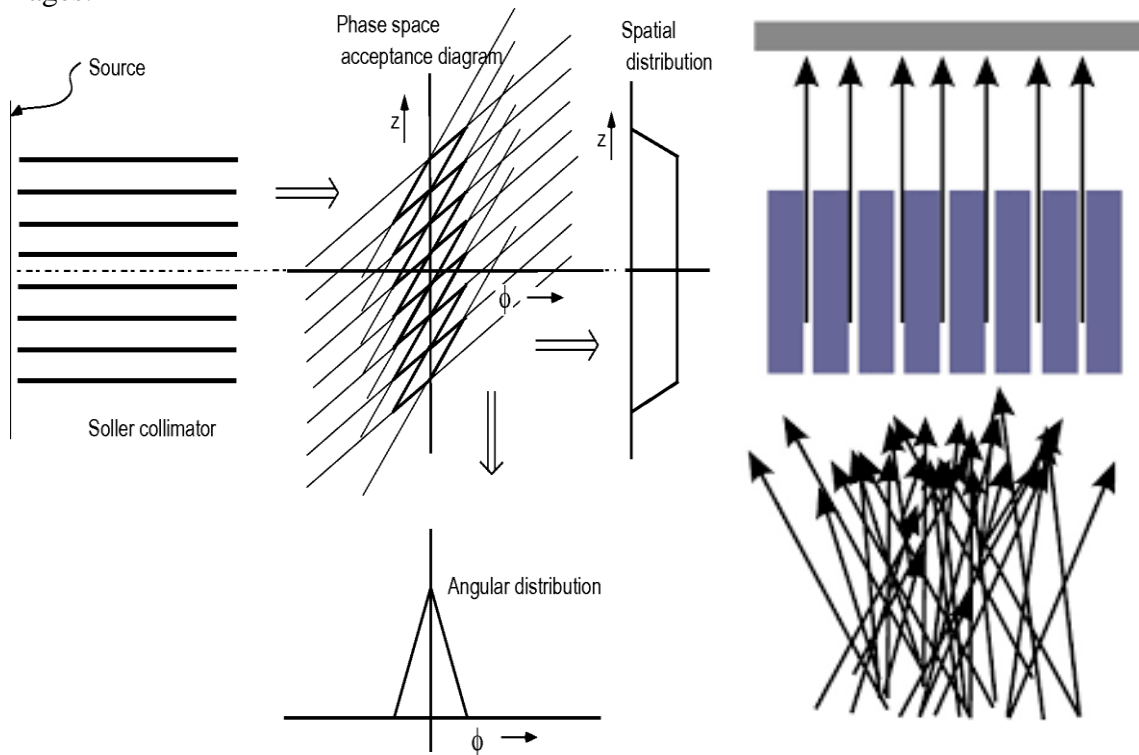


Figure 4.7: Schematic Soller collimator with vertical channels and its optical transmission properties



Figure 4.8: Focusing collimator used in neutron experiments

However, we have used our collimator before the sample and sample environment in order to achieve the splitting of our neutron beam in 5 distinct channels. This utilization of radial collimators is also called focusing collimators, as it is used to focus the beam (5 channel multibeam in our case).

So our system consists of the elliptical focusing guide, which is bent in horizontal direction and the system of collimators for achieving the multibeam distribution.

Below there are the 2D plots of the multibeam intensity distribution after the splitting into 5 sub-beams by the horizontal channels. Note that at the focus spot, there is only one peak visible from the beam, which is a clear sign that there is no cross-talk between the sub-beams.

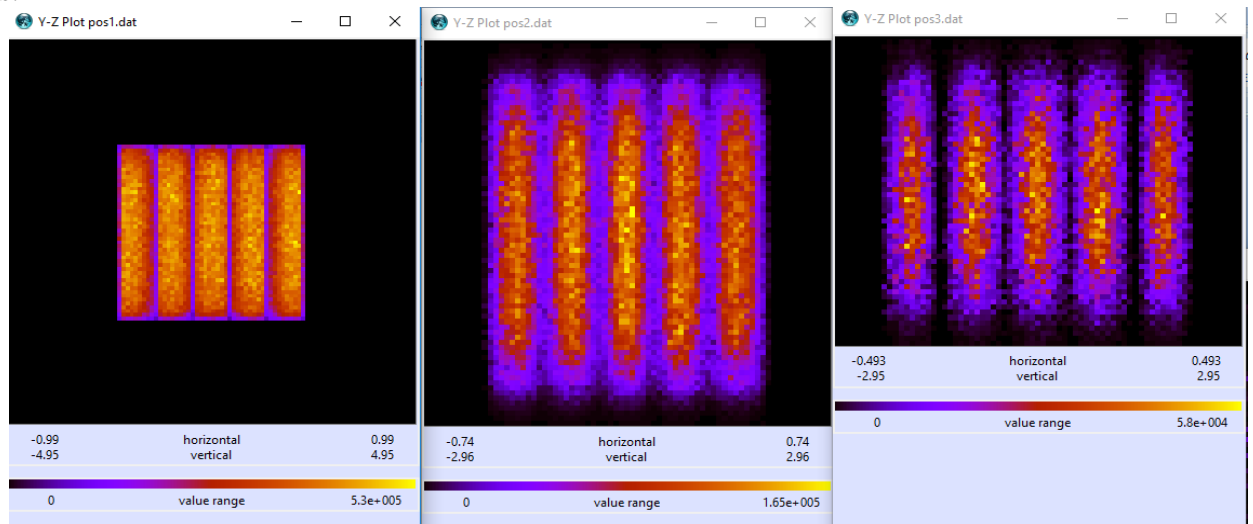


Figure 4.9: 2D Intensity distribution of the collimator system- the first is the distribution after the first collimator; the second is after the 3rd collimators and the third is after the collimator system before the focus

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5. Conclusions and discussions

We have conceived and designed the neutron optic system of the new neutron source and reflectometer (spectrometer) which will be developed in the near future (in the next years) and built in the far future at the Joint Institute for Nuclear Research (JINR), in Dubna, Moscow Region, Russian Federation. We have as well performed simulation experiments for assessing the optimal configuration and parameters for this installation, based on the current knowledge about the properties of the neutron source and the radiation field.

According to the literature, theoretical works and textbooks presented in the previous chapters and by the gained valuable experience from our results, the most optimal configuration for neutrons of low wavelength (0.5-1.5 Å) is the linearly decreasing guide, while for the neutron of higher wavelength (2 -15 Å) the elliptical focusing is preferable, with higher guide exit compared to the entrance. Comparison graphs and plots were presented in the previous sections, as well as the advantages and disadvantages of the different systems, both from principle point of view and from technical realization difficulties.

Besides the focusing part, a multibeam illumination system was designed and tested, using radial and soller collimators to divide the neutron beam in 5 sub-beams and to prevent crosstalk between these from the guide exit to the sample and detectors. This division into 5 different sub-beams is essential to cover a much higher Q-range (the momentum difference of the neutron interacting with the sample) in order to be able to study wide range of phenomena, both in the case of biological soft matter and of solid state physics.

Our instrument suite proposed to be built also takes into account the engineering and technical difficulties and challenges in the way that the presented design is easy to build, maintain and it is the cheapest option for the given performance requirements.

As the project for the new neutron source evolves in time, a more precise and detailed technical analysis will be required, based on the current work and on the exact physical and radiation characteristics of the new source, which are not fully known yet. According to these, the present work will be the base and starting point for the new ambitious project at JINR.

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