Optimizing the neutronic performance of the NMX instrument at ESS, the world's brightest neutron source

To be able to tailor medical drugs to specific proteins it is important to know the inner atomic structure of the protein. This is one of the usages of the information that will be collected at the future brightest neutron source, ESS, being built in Lund.

Currently a new, world leading scientific facility is being built in Sweden, called ESS. At ESS, they will use neutrons to perform many different kinds of experiments. To perform the different experiments instruments will be connected to the core of ESS, where neutrons are released. One of the experiments that will be performed is to shoot a beam of neutrons at a protein crystal. This experiment will be performed at an instrument called NMX. When the neutron beam hits the protein some of the neutrons will bounce of the atoms of the protein. Depending on the distance between the atoms within the protein the neutrons will bounce in different manners. By looking at how the neutrons have bounced it is possible to extract information regarding the inner structure of the protein. This information may then be used to tailor medical drugs to match specific proteins.

To be able to perform the experiment described above, the neutron beam has to be guided from the core of ESS out to the protein. During the transport of the neutrons from the core to the protein the properties of the neutron beam are decided. Mainly two properties of the beam are of interest, the cross section size (how big it is) and the divergence (how much the neutrons spread out).

To control the size and divergence of the neutron beam, the beam passes through two aligned apertures. An aperture, in this context, is basically a plate made out of material that easily absorbs neutrons, with a hole in it where the neutrons may pass. Neutrons that have wrong positions in the beam or a wrong divergence will not be able to pass through the apertures but will instead be absorbed by the plate. Changing the size of the apertures enables these properties to be selected in a desired range. It is important to control the properties to match the different protein samples that are examined. For example, as the proteins are kept in a liquid, if a neutron hit the liquid instead of the protein it is likely to bounce of the atoms in the liquid, which will impair the result of the experiment. The system that contains the two apertures defining the size and divergence of the neutron beam at NMX is called the Beam Geometry Conditioning System.

The most important aperture is the one closest to the protein. This aperture defines the cross section size of the neutron beam. To obtain the best result of the experiment the distance between the protein and this aperture should be as small as possible. At the same time, the material surrounding the aperture must not obscure too many of the neutrons that have bounced off the protein. The design of this aperture is key to the functionality of the entire instrument and tradeoffs have to be made. The closer to the protein the aperture is the better quality of the neutron beam reaching the protein, but, at the same time, more bounced neutrons will be blocked.

Many different designs of this aperture have been investigated to find the best solution. To compare the different solutions they were scored on a number of different criteria. Based on the scoring, the best solution was found.

The best design (Fig. 1) consists of an absorber shaped like a cartridge with a fixed aperture size. The cartridge is kept in place on a mechanical arm using magnets. By using magnets, the cartridge may easily be replaced with another cartridge, with another aperture size. Up to ten passive cartridges are stored in a carousel next to the arm. Exchanging the active cartridge to one of the passive ones is done automatically using a stepper motor and two pneumatic stages.

The benefit of this design is that the tip of the cartridge is very small and may be placed very close to the protein while not obscuring any bounced neutrons.

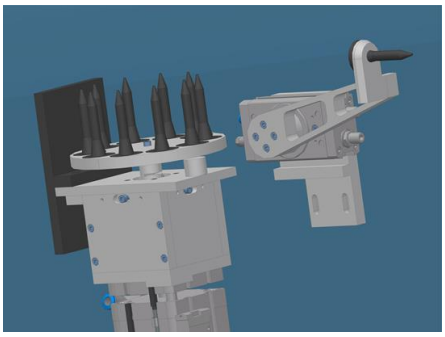

Figure 1: Design of the aperture closest to the protein

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