Feasibility of Using a Small Angle Neutron Scattering Beamport with an eVinci Hybrid University Research and Power Reactor

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Abstract

This project is a preliminary investigation into using the eVinci micro power reactor as a neutron source for a university-based Small Angle Scattering (SANS) instrument. This was done by using the program McStas to simulate neutron scattering. Due to time constraints as well as neutron intensity and budget concerns, thermal neutrons were used. Due to the use of thermal neutrons, single crystal monochromatization was used by simulating a BeO crystal mosaic. The sample used to determine the viability of the setup was SANS_spheres2, and this gave us a Q range from approximately 0.1-0.01 Å^{-1}. Although these early results were promising for a lab-based SANS instrument, further investigation relating to more accurate intensity and crystal simulations must follow our work.

Acknowledgements:

There are significant contributors to this project to whom we would like to give thanks. We had the special opportunity to meet and learn from the instrument scientists at NIST, John Barker and Tyler Martin. Norbert Hugger gave us invaluable insight for understanding and learning about MCNP as well as general advisement on the project. Last but certainly not least, Professor David C. Medich acted as our primary counsel and mentor on the project and helped most significantly in its guidance and direction.

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1. Introduction

Nuclear fission reactors generally are either designated as research reactors or power reactors. The Westinghouse Electric Corporation has designed the generation-IV eVinci microreactor, which has a maximum power output of 5 megawatts electric (MWe) when producing its rated 15 megawatts of thermal energy (MWt). This eVinci microreactor is designed to be a small power reactor, but eVinci's output puts it in line with currently operational university research reactors, which generally work with power outputs as high as 20-80 MWt. Yet current research reactors are based on technology dating back to the 1950s and 60s and are not designed to also produce electricity. As a next-generation power-producing microreactor, the eVinci is also designed to be conveniently transportable and has passive safety systems while also retaining relatively reasonable economic feasibility. This makes it much safer than current reactors and suitable for deployment in environments with low to middle level energy needs, such as Worcester Polytechnic Institute [1].

The combination of it operating at thermal energies equivalent to current upper range research reactors coupled with the ability to meet WPI's energy needs has prompted us to consider the possibility of adapting eVinci to take on the functionality of a hybrid research and power reactor. As mentioned, eVinci's thermal power output is comparable to that required of designated research reactors; simultaneously, eVinci's electrical power output of 5 MW is sufficient to supply a small-footprint environment such as a small university campus with its energy needs. As an example, our own Worcester Polytechnic Institute's (WPI) energy requirements averaged out to 2.8 MWe in the 2020 fiscal year, peaking at 4.1 MWe.[1] In that case eVinci could then reliably provide adequate and sufficient power to infrastructure, while also being able to provide the power needs for potential research. Research utilizing neutrons is a potential benefactor of eVinci's hybrid functionality, as a substantial amount of neutrons are produced in the eVinci reactor core because of its operation. Specifically, we investigate the potential feasibility of Small-Angle Neutron Scattering (SANS) research using the eVinci as a neutron source in this project.

SANS is an imaging technique that relies on the measurement of the angles at which a narrow beam of neutrons scatters when passing through a sample. The 2D or 1D pattern that results at the detector reveals information about the molecular, structural, and isotopic features of a sample. It is essential that the energy/wavelength of the neutrons is known when they hit the sample since the scattering angle is dependent on neutron energy/wavelength.

Many laboratories around the world have scattering instruments (e.g., SANS) that use research reactor neutron sources. The technique of scattering allows for the imaging of very small structures to incredibly fine resolutions, using x-ray radiation (SAXS) or neutrons (SANS). For imaging via radiation scattering, either type of radiation can be segregated from the core of a reactor via one of (typically) several beamports funneling radiation directly into these scattering instruments, providing a high-volume and steady source of neutrons or x-rays. This has wide application in the imaging of various materials and compounds in the fields of microbiology, polymer science, atomic spectroscopy, and complex fluids.

SAXS obtains information at the atomic level, since X-rays are absorbed or scattered by atomic electrons; neutrons interact with the nuclei of atoms and therefore can be used to probe even smaller structures than x-rays [1]. SANS is generally used to probe structures on length scales from micrometers down to nanometers. This has We wanted to see what a potential SANS instrument would/could look like with eVinci, and how it would perform. To that end, we employed MCNP ("Monte-Carlo Neutral Particle," which is based on the Monte-Carlo computational methods) software to create virtual instances that simulate such scenarios. However, while MCNP is a general-purpose tool, it is not as specialized or optimized for what we wished to do. This led us to discover McStas, another Monte-Carlo-based software that is specifically designed to simulate neutron scattering. MCNP was developed by Los Alamos National Laboratory, but MCSTAS has been actively supported by a handful of international laboratories with reactor neutron sources and SANS instruments such as those of ILL and ESS, and is available for free use via the website mcstas.org. MCSTAS became the primary software and means in this project for constructing virtual SANS instruments and simulating SANS scenarios. We hypothesize that applying eVinci as a hybrid research reactor, in addition to retaining its power reactor functionality (5MW electric, 15 MW thermal), can make SANS research more accessible to a greater number of facilities, while also providing a source of power to those facilities.

TABLE 1: SELECT LIST OF INTERNATIONAL CONTINUOUS SOURCE RESEARCH REACTORS WITH ACCOMPANYING SANS INSTRUMENTS [2]

Neutron Reactor Source	SANS neutron energy range	Maximum Thermal Power Output	Location
HFIR	cold	100 MW	Oak Ridge (TN), USA
NIST	cold	20 MW	Gaithersburg (MD), USA
MURR	thermal	10 MW	Columbia (MO), USA
Risø	cold	10 MW	Roskilde, Denmark
ILL	cold	57 MW	Grenoble, France
CMRR	thermal	20 MW	Mianyang, China
Dhruva	cold	100 MW	Mumbai (Bombay), India
MNR	thermal	5 MW	Ontario, Canada

2. Background

2.1. Typical SANS Instruments

A typical SANS instrument has a few major components, those being the source, velocity selector, collimator, sample, and detector. The source is where the neutron beam originates, and is defined in terms of parameters that dictate the way the neutrons are propagated in space, such as their mode and pattern (e.g., planar, isotropic, etc.). SANS devices often operate with cold neutrons, which can come from a fusion reactor and can be cooled using liquid hydrogen. However, this is not always the case since pulse sources are also used in some cases.

Neutrons must have a known particular energy to be able to obtain any useful information from their interactions; i.e., the beam of neutrons must be monochromatized. This can be accomplished by two primary methods: through usage of a velocity selector component or a time-of-flight (TOF) method. A velocity selector is a device that contains series of rotating disks which only allow neutrons of a specific velocity (and therefore also a specific energy/wavelength) to pass through and exit out the other side. This produces a somewhat constant beam of monoenergetic (alternatively, "monochromatic") neutrons to hit our sample. The time-of-flight method involves a pulsed beam that determines the energy of the neutrons based on when they hit the detector, such that scattering angles become time-dependent and, by extension, wavelength.

After passing through the velocity selector, the neutrons must then be focused into a small laser-like beam. This is commonly done by pinhole collimation via two small holes a distance apart. Finally, the neutron beam interacts with the sample and scatters. This scattered beam then reaches the detector, where there are many individual detectors that are each pixels in a grid, so that complex scattering patterns can be analyzed. To reduce costs, some labs have a 1D detector where only the average intensity with relation to radius is measured. [3]

2.2. Q value

The Q value (or simply just Q) is a parameter used to describe the scattering angles, limits, and resolution of a SANS device. It is a wavelength-independent scattering angle that can be used to compare results even if the measurements are made using different wavelengths. Q is represented by the equation

$$Q = \frac{4\pi}{\lambda} \sin\left(\frac{\theta}{2}\right) \tag{1}$$

Where the angle of the beam from the center of the detector is represented by θ and the wavelength of the beam itself is represented by λ. The unit for Q is generally $Å^{-1}$ as the wavelength is measured in Å. SANS devices often can compare certain parameters relating to Q to find out what they can and cannot measure, these being the minimum and maximum Q values as well as the resolution of that measurement called dQ. Minimum Q is dependent on the spot size of the beam with no sample present. In a system using pinhole collimation this can be calculated using the distance between both holes, the sizes of the holes, and the distance to the detector. The spot is normally blocked by a beamstop; even if there was no beamstop, the unscattered beam intensity dominates over that of the scattered neutrons in this region. The maximum Q can be found by the distance between the sample and the detector as well as the size of the detector, so a detector really close to the sample would, in theory, have a higher maximum Q compared to a detector of the same size further away. In practice, due to background noise less neutrons scattering at larger angles, and a larger area the neutrons are spread over, size is not the only limiting factor for maximum Q realistically. Finally, dQ[2] is one of the more complex quantities of a SANS device to calculate as it depends on many factors. It is the minimum difference between Q values that can measured and is dependent on the detector ‘pixel’ size, the wavelength spread, the angle of scattering, and the geometry of the SANS device. The wavelength spread can be calculated using the equation

$$\frac{\Delta\lambda}{\lambda} = \lambda_{spread} \tag{2}$$

Where $\Delta\lambda$ is the full width half maximum of the distribution of neutron wavelengths and λ is the mean wavelength. This value is often given as a percentage.

2.3. Neutron Energy Spectrum

During reactor operations, the nuclei in the core undergo highly energetic nuclear reactions, leading to many particle emissions. These emissions are not monochromatic; there are neutrons of several energies as well as other non-particulate radiations (namely gamma rays) coming out of the reactor core. As explained in Section 2.1, the scattering instruments do not make use of the wide variance in radiation energies coming from the reactor core, but instead rely on incident radiation being monochromatic. SANS instruments at different reactors around the world most typically operate with "thermal" or "cold" neutrons (we observed a tendency for the latter, generally speaking). These terms refer to their energies/wavelengths on the neutron spectrum, in addition to other types such as fast neutrons and epithermal neutrons. These other neutrons must be filtered out for the proper operation of the SANS devices. The neutrons on the aggregate can then be distinguished based on their kinetic energy, which is correlated with their speeds and therefore to their deBroglie wavelengths.

TABLE 2: SPECTRUM OF NEUTRON ENERGIES BY WAVELENGTH [4]

Range	Energy (eV)	Wavelength (Angstroms)
Cold	<0.025	> 1.81 (typically 4+)
Thermal	0.025	1.81
Epithermal	0.025 - 1	0.286 - 1.81

Slow	1 - 10	0.0904 - 0.286
Intermediate	10 – 10^6	2.86 x 10^{-4} - 0.0904
Fast	> 10^6 (1 MeV)	< 2.86 x 10^{-4}

This filtration process inevitably also reduces the total number of particles entering the instrument, thus reducing the flux observed at the detector of the apparatus.

Early in the project, we decided that thermal neutrons (wavelength roughly 1.8-2 Å) would optimal for type of SANS setup we envisioned, as opposed to the more standard colder neutrons (4+ Å). This was for three reasons, the first being cost: not needing the equipment to bring neutrons down to cold energies could dramatically reduce cost and complexity (liquid cold moderators like hydrogen and deuterium are more costly to use, and in some cases pose as hazards). The second reason is the time constraint of this project, as simulating and designing a cold source for the reactor would be too large of an undertaking. The third and final reason was to increase the neutron intensity hitting the sample; a cold source would absorb more neutrons.

3. Methods

3.1. MCNP and early calculations

In the beginning we planned to use MCNP to simulate the SANS instrument and figure out how feasible it was and what resolutions could be achieved. Yet early on there was a roadblock: because of MCNP's homogeneous methods for neutron simulation, crystal structures and neutron scattering could not be simulated. For SANS experiments, it was clear that we could not rely on it for most of our calculation and simulation needs. At this same time, MATLAB was used to program a Q-value calculator, that would take all the parameters as an input and then output the theoretical minimum Q and dQ values based on geometry and wavelength spread. This became useful later since a flux from the reactor could be provided; rough calculations could be made as to what the flux would be at the sample, then the program could be used to work backwards by getting the desired neutrons per second to figure out what the resolution would be like at the detector. The program could also be used to optimize the beam stop size. A popular SANS benchmarking test involves the use of small polystyrene spheres submerged in (in our case) heavy water as it can show the amount of smearing that will occur in the output [5]. The scattering pattern of spheres can be represented by the equation

$$P(Q) = \left[\left(\frac{3}{QR}\right)\left(\frac{\sin(QR)}{(QR)^2} - \frac{\cos(QR)}{QR}\right)\right]^2 \tag{3}$$

Where R represents the radius of the spheres, Q represents the Q value as mentioned above, and P(Q) is the relative intensity. This equation does not account for factors that affect the output like smearing, yet it gives a good idea of how much information you can expect between your device's minimum Q and maximum Q values. The spheres equation (and its inclusion in the simulation) is incredibly helpful for troubleshooting McStas simulations, as it can be to check if the beamstop is too large, the detector is too small, or if it is a separate problem all together.

3.2. McStas

Because of the limitations of MCNP, we decided to use a program called McStas (Monte Carlo Simulation of Triple Axis Spectroscopy). This neutron imaging simulations program is found online at https://www.mcstas.org/ and is specifically designed to model SANS, neutron spectroscopy setups, and other neutron scattering environments. An instrument in McStas can be built with several premade or custom components that can easily be positioned along a beamline. McStas does have its drawbacks, although it is good for getting an idea of what an output from a SANS instrument may look like. It relies heavily on needing a lot of information given to it and it is difficult to get good data out of it. For example, the methods to find neutron intensity and/or absorption are much of the time either interpolated data from MCNP (if you are lucky) or an approximation. It’s good enough for figuring out scattering results yet.

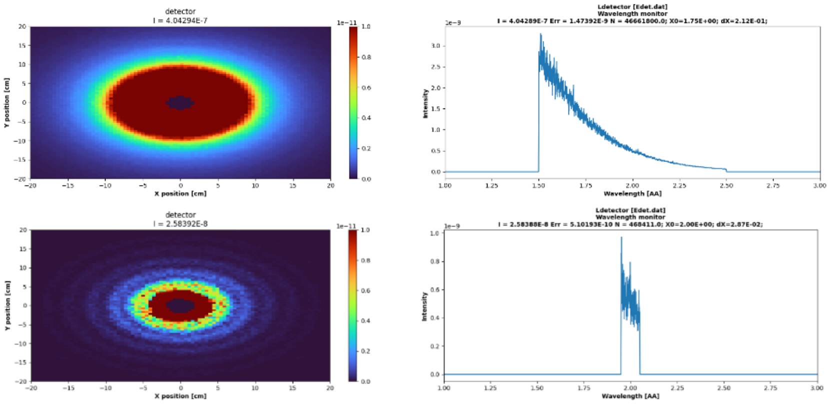

Figure 1: This shows the differences between a 5% and 50% wavelength spread for a 2AA beam.

One of the first tasks we accomplished with McStas was combining two simple setups: A crystal monochromator and a simple SANS setup, the main components consisting of a source with a gaussian distribution, a single crystal filter, a pinhole collimator, a sans spheres sample, and a 2D detector. Due to McStas having a simple-to-use coordinate system allowing for objects to be placed relative to one another, combining these two systems turned out to be quite simple. Yet when we ran the simulations, we noticed that our neutron intensity values were quite low. The decision was made to use a simple SANS setup to track down the issue where the source was a perfect laser beam hitting the sans spheres and scattering onto a 2D detector. We found the same very low intensity measurements during this process, so it was decided to take apart the source code line by line to see how this output was justified. What was found was a very ‘theoretical’ output that was found to be too much of an approximation, so another test was run with Sans spheres 2 that gave a much more realistic output that was more in line with reality. This included a much more believable intensity as well as the simulation accounting for background/incoherent scattering in the higher Q regions.

3.3. Monochromatizating

As discussed in Section 2.1, monochromatization of a neutron beam can be attained using a velocity selector component (commonly with continuous cold sources) or a time of flight (ToF) method (commonly with pulsed sources). SANS setups working with cold neutrons typically opt for incorporating velocity selectors as they do not alter the direction of the incident neutron beam, and typically result in a wavelength spread >10% [3]. There is, however, a third alternative method for monochromatization. Crystal monochromators see use in a number of SANS instruments that operate with thermal neutrons, like that of the 100 MW Dhruva research reactor, which contains a Beryllium Oxide (BeO) crystal. Crystal monochromators can be more optimal for working with thermal neutrons than velocity selectors, but are generally not favored over velocity selectors since crystal monochromatization involves redirecting the neutron beam. However, crystals can achieve significantly lower wavelength spreads in the range of 1-5%.

Early on it was realized that the neutron energy would be so high that a ~20% variation in wavelength would have a substantial impact on our dQ value, smearing the data beyond a usable point. This put a mechanical velocity selector out of the question for our purposes as they have larger wavelength spreads with decreasing wavelength. This left us with essentially only one option: using a crystal monochromator. They are not used in most SANS setups since they only work at wavelengths up to 3Å. A crystal filter would consist of a single mosaic crystal precisely angled and with a specific crystal structure such that, due to Bragg scattering, neutrons of the desired wavelength are scattered into the pinhole collimator. This can be simulated in McStas using a few methods, the simplest of which is to use the single crystal component. There are however other methods, like an add-on called NCrystal. Unfortunately, we did not have the time to incorporate NCrystal, yet it can yield much more accurate results for spectrum and reflected intensity results.

Much research was put into the crystal filtration component due to the importance of having a monochromatic beam with a lower wavelength spread than what would be allowed on a cold neutron SANS device. We were advised to consider using BeO crystals due to the spectrum of neutrons we were dealing with, although many more alternatives were found through research [6]. It was decided that we should stick to BeO as spending time optimizing crystal material was outside the scope and time constraint of this project.

3.4. Using SANS_Spheres2

Eventually the component SANS_Spheres2 was used to provide a more realistic output that gives more realistic values for background and incoherent scattering as well as more realistic intensity values at the detector. When we ran SANS_Spheres2 in our simplified setup with a perfect beam source and nothing else besides the sample and detector, we observed the expected pattern. When this was then put into the complete SANS instrument (wider energy spectrum from source, single crystal monochromator, pinhole collimator, sample, then detector), that pattern was not apparent. It was then realized that between SANS_Spheres2 and the original Sans_spheres, one value had a unit change, causing the excess scattering length density to be off by a factor of 10E+11. This was quickly fixed, and the simulations ran after showed the typical sphere scattering pattern.

4. Results

4.1. McStas

The first McStas result we successfully ran showed the output from a single crystal monochromator. Once the SANS component was added we obtained the expected results: concentric rings of neutron intensity. However, if you note the intensity post-monochromatization, the beam peaks at 1e-07 n/(s*cm^2) and the reading at the 2D detector (named "detector") peaks around 4e-23. In one test where we had a simple perfect beam source and our sample, the source intensity was 7e+08, and the detector intensity was around 10e-61. This immediately set off some red flags, as a less-than-centimeter-thick piece of heavy water and plastic beads could not decrease neutron intensity by around 1e+69. Digging through the Sans_Spheres code and breaking apart the calculations showed that, although it's a good demonstrator of the resolution of the device, it was a poor calculator of intensity and incoherent scattering as that was mainly handled through rough approximations. This made the resulting Q range unrealistically high.

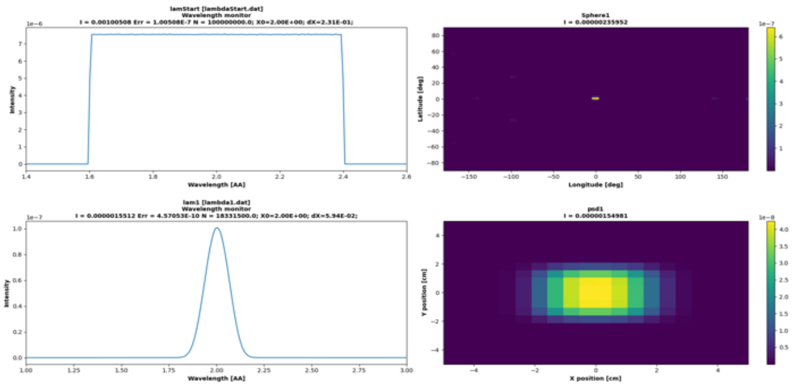

Figure 2: First output from McStas showing a single crystal monochromator.

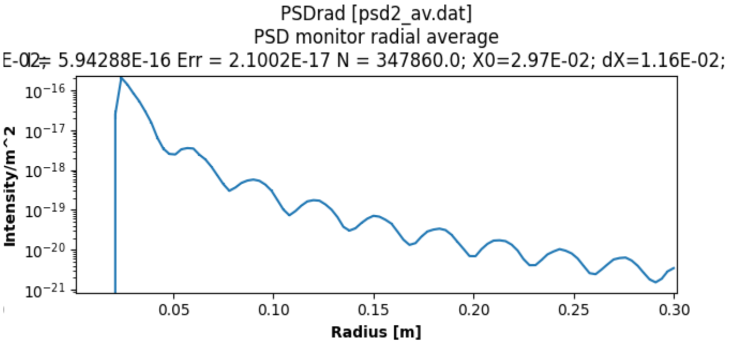

Figure 3: This graph from McStas shows the results from using SANS_spheres

4.2. Sans spheres 2

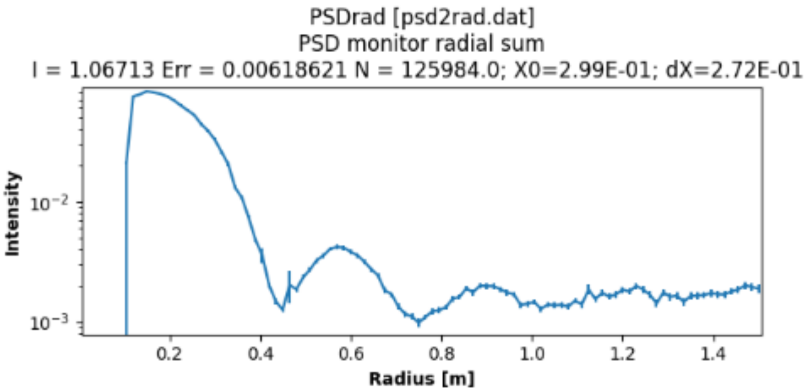

FIGURE 4: INTENSITY VS RADIUS GRAPH TAKEN FROM MCSTAS SHOWING THE RESULT FROM SAMPLING SANS_SPHERES2

After we switched to SANS spheres 2 and put it in the simplified setup consisting of just a source and sample, we immediately saw only around a 1e03 reduction in intensity, that is much more in line with what is expected due to the larger area the neutrons are spread out over, as well as the fact that neutrons that don't get scattered get absorbed into the beamstop. In this model you can see background/incoherent scatterering dominate past the 0.1m mark. In the original Sans Sphere model, the oscillating pattern continues out constantly decreasing, yet still clearly identified and gave a much wider Q range than what was realistic for our setup.

When SANS_Spheres2 is placed into the full simulated SANS setup that includes the gaussian source, crystal monochromator, and pinhole collimators a more realistic result is produced (Figure

4). With this setup, a maximum Q value of approximately 0.1 $Å^{-1}$ was obtained before noise drowned out the signal. This sample had the spheres set to a radius of 100 Å.

The wavelength spread for these trails is better than what was expected, being 4.8% right after the crystal and 1.2% right before the sample. This is a smaller wavelength spread than what was simulated in the simplified setups, as for those trials we estimated it to be 5%.

5. Analysis

5.1. Wavelength Spread

Using MATLAB, we were able to calculate the $\Delta\lambda/\lambda$ values for our beam shortly after the crystal and at the sample itself. We found that the spread was 4.8% right after the crystal and 1.2% at the sample, this is a lot better than I was expecting as the rough estimate we made when doing our preliminary calculations was that the spread would be around 5%. This result could however be due the default crystal data not being fully realistic and the fact that they do not contain the imperfections that would exist in a real word crystal; however the long length of our collimator would aid in removing the neutrons that scattered off at a different angle.

5.2. Q range

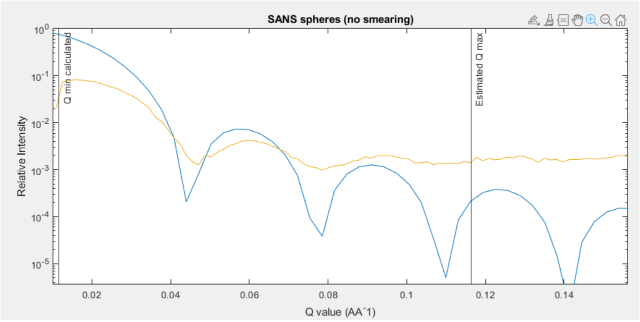

FIGURE 5: THIS GRAPH REPRESENTS THE SIMULATED INTENSITY (YELLOW) AND THE CALCULATED INTENSITY (BLUE)[8]

From Figure 5 the blue line shows the calculated intensity and the yellow line shows simulated intensity. The calculated line does not consider smearing from resolution, the noise floor, or the minimum Q value. Hence why the simulated line has so much variation, despite this, a clear correlation is shown with the location of the peaks and troughs aligning. It's the width of these peaks that allows the structure of this sample to be determined, and thus showing that it can produce distinct and useful results. With our data, we were able to calculate a reasonable estimated Q-range of roughly 0.006 - 0.1 Å^{-1}. Although this does not exceed the ranges of current state-of-the-art SANS instruments, it is more than viable and comparable to an accessible lab-based SANS device. This, however, is still a relatively rough simulation and most likely a more liberal range and resolution calculation and is expected to decrease when more accurate crystal and transport simulations are performed.

5.3. Error Analysis

The error for our simulated intensity, although present, is thought to be negligible compared to the unknown values presented from neutron transport and crystal simulations when compared with better methods of simulation. Given that the cross sections used by McStas typically have a relative uncertainty of about 2% and that inherent variations in the ray-tracing aspects of McStas (I.e. the non Monte Carlo aspects of this code), may have anywhere from 10-20% relative uncertainty, we approximate our results to have an uncertainty of approximately 20%.

6. Future Work

6.1. Cold Neutrons, USANS, and Neutron Spectroscopy

Our work simulated neutrons around the thermal spectrum, having wavelengths ranging around 1.8-2Å. Most SANS setups use wavelengths ranging from 4-12Å, this however requires a cold source attached to the reactor. Designing and then using MCNP to simulate the flux from a cold source attached to our reactor would be particularly insightful.

Going the other direction on the energy spectrum we have USANS (Ultra Small Angle Neutron Scattering) and Neutron spectroscopy that use smaller wavelength neutrons yet typically have different methods for detecting scattering angles.

6.2. NCrystal and MCNP

Using more accurate simulation methods to get better data for the neutron intensity and crystal reflections are almost necessary if this project is to be considered beyond what we have.

MCNP could be used in scenarios where no significant neutron scattering occurs to more accurately predict what neutron intensities we could expect at the sample. MCNP would also allow the neutron energy spectrum to be more accurately predicted as the energy loss from neutron interaction due to various levels of vacuum and neutrons leaking through the collimator could cause the 1.2% wavelength spread to broaden. The simulation also does not account for secondary radiations caused by any of the neutron interactions that also affect the noise floor.

NCrystal is a software package for modeling thermal neutrons in crystals and is compatible with a variety of simulation programs including McStas and geant4. NCrystal would allow for a more realistic model to be made when it comes to the neutrons that are Bragg scattered vs those that are absorbed or scattered incoherently.

6.3. Material and Geometry Optimizations

The single crystal setup could be improved in many ways. The specific mosaic pattern, material, and thickness could all be optimized to improve wavelength spread as well as increasing neutron intensity and the ratio reflected for a specific wavelength. Asymmetric reflections, a method that can increase the beam intensity by reflecting the beam in such a way that the beam dimensions get compressed[7], could also be researched as a potential way to make this device more versatile. In our simulation we used a single crystal filter, however some other setups make use of a double or even triple crystal filter setup. The type of crystal can also change: we used Beryllium Oxide, yet the industry commonly uses Si 111, there are also many alternatives being researched using materials such as diamonds.

Other things to consider going forward includes the macroscopic geometry of the instrument. Adjusting variables such as the length of the system overall as well as the ratio between the length from the crystal to the sample and the sample to the detector. The radius of the apertures on the pinhole collimator can also be adjusted to allow for more intensity at the cost of less resolution and a larger minimum Q, finding the optimal balance between these two would yield lower count times and potentially a lower noise floor.

7. Conclusions

So far, these results are promising. Although our SANS setup would not be as accurate as many of the research leaders out there, it still would be a huge advancement in the accessibility of this instrument. SANS would go from being a technique implemented only at large designated research reactors to something that a small-to-midsized university can install and utilize. It will not revolutionize imaging in the sense that it does something that nothing else can, but it will be productive by paving the way for increased accessibility and lower costs associated with SANS-based research. Having access to an average device is better than not having access to any device at all. It is our hopes that through the results produced in this project, we have put SANS into the realm of possibility for a facility using the eVinci microreactor as a neutron source. The groundwork has also been laid for thermal neutron SANS devices going forward in respects to monochromatization methods and expected range. Having painted a picture of potential feasibility, we look forward to implementation and optimization as the next steps for SANS with eVinci.

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