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Performance Gain with Low-Enriched Fuel and Optimized Use of Neutrons

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Abstract

The most challenging type of reactors to convert to low-enriched fuel are high-flux research reactors, which, along with some spallation sources, are the most important neutron sources for modern neutron scattering experiments. Advanced Monte-Carlo computer codes are now available that make it possible to track neutrons from the reactor core, through neutron guides, to instruments and detectors. These "virtual experiments" allow optimizing the performance of a research facility as a whole instead of the reactor alone. This article briefly reviews performance gains obtained for high-flux reactors during previous facility-upgrades. The Monte-Carlo code VITESS is used to compare results for typical neutron scattering experiments using obsolete versus state-of-the-art technologies. The analysis shows that performance gains due to instrument upgrades or neutron guide renewals dwarf potential neutron flux losses due to conversion to low-enriched fuel. Combined convert-and-upgrade strategies therefore offer unique opportunities for reactor operators and neutron instrument groups to significantly improve the overall performance of research facilities.

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Background

International efforts to convert research reactors that are fueled with weapon-grade highly enriched uranium (HEU) to low-enriched fuel have intensified significantly since 2002. In addition, new high-density low-enriched fuels are now under development in the framework of the RERTR program. These fuels could be qualified within the next years and will offer an unprecedented opportunity to end the use of HEU in the civilian nuclear fuel cycle entirely. Even the remaining HEU-fueled high-flux reactors, which are the main facilities used for neutron-beam research today and account for about half of the total HEU-demand worldwide,[1] could then use low-enriched fuel.

When transitioning from HEU to LEU, however, reductions of the neutron flux on the order of 10–15% are sometimes inevitable—especially if the original reactor was designed for HEU, and design modifications of the core are constrained. The INFCE criteria had already emphasized in 1980 that *"neither any loss in the overall reactor performance (e.g. flux per unit power) nor any increase in operation costs should be more than marginal."*[2] Predictably, arguments in favor or against conversion of a particular facility often revolve around what constitutes an acceptable "marginal loss" of scientific usability of a reactor. Yet, the maximum neutron flux near the core is only one quantity to characterize facility performance. In the case of high-flux reactors, the effective neutron intensity at the *sample or detector position* is critical instead. Hence, in order to obtain an accurate assessment of the conversion process, which can be combined with an upgrade of neutron guides and instruments, so-called "virtual experiments" can be a vital tool.

Virtual experiments model the path of the neutrons from the source near the reactor core through a neutron guide to the sample and the instrument. They play an increasingly important role in designing and optimizing modern neutron-scattering instruments.[3] As this analysis shows, virtual experiments can—and should—also play an important role in evaluating the conversion options for research reactors and in optimally allocating the available resources.

Virtual Experiments

The results presented below are based on simulations with VITESS (Virtual Instrumentation Tool for the ESS), which is a Monte Carlo neutron transport code for neutron scattering at pulsed and continuous neutron sources.[4] Originally developed for the instrument-design of the European Spallation Source, VITESS has since evolved into a flexible code-system that is actively used on a series of neutron instruments worldwide and has been extensively tested and validated over the last years.[5] Tallied quantities include neutron intensity, divergence, spectrum, polarisation, and others. As an example, Figure 1 shows typical results of simulations that will be discussed and analyzed further below.

For the present analysis, a generic and rather simple setup is modeled because only the effectiveness of propagating neutrons through the guide is of interest here. As the reference source for all simulations, we use the spectrum of the cold neutron source of the High-Flux Reactor at the *Institut Laue Langevin* (ILL), which is provided as a default data set with VITESS. The neutrons enter the guide at a distance of 200 cm from the source.[6] The guide-module then simulates the neutron flight-path through the mirrored guide calculating the intensity loss for each reflection as a function of the neutron wavelength and incident angle.

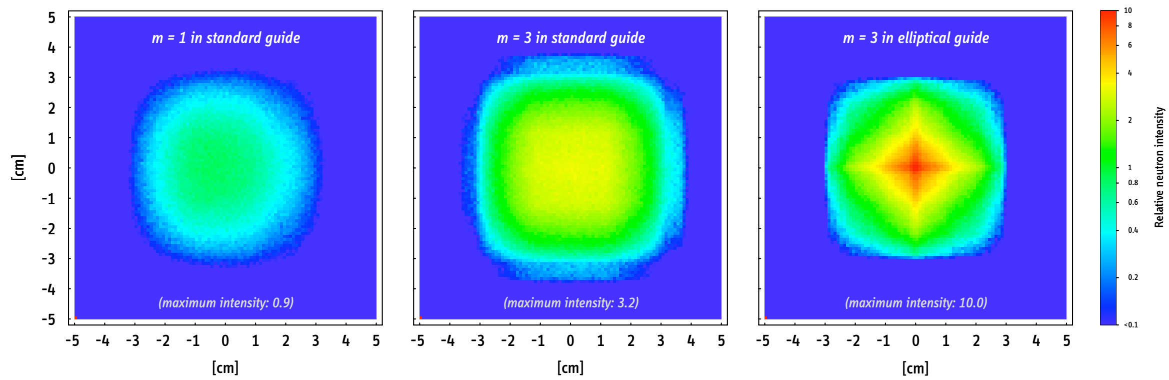

Figure 1: Spatial intensity distributions for selected supermirror coatings and two guide geometries that will be discussed in the analysis below. Shown are the planes of best focus behind the exit of a guide with a total length of 35 m. Each simulation is based on 10 million neutron tracks.

Results

We explore two basic options to optimize cold-neutron propagation through the guide: advanced supermirrors and innovative neutron-guide geometries. Simulation parameters and conditions at the front-end of the setup, i.e., from the source to the guide entrance, remain unchanged in all cases. The neutron wavelength and spatial intensity distribution (as shown in Figure 1) of the neutron beam are then monitored at several distances from the exit of the guide.

Advanced Supermirrors

In order to optimize propagation of neutrons through a guide, the critical angle for total reflection has to be as large as possible. In general, this angle is given by:

$$\theta_c(\lambda) = \sqrt{\frac{N\,b}{\pi}}\,\lambda$$

Here, N is the number density and b the scattering length of the material. For natural nickel, the element with highest value for $N\,b$, $\theta_c(\lambda) \approx 0.099^\circ\,\lambda(\text{Å})/\text{Å}$. Supermirrors "artificially" increase the critical angle through a large number of thin, depth-graded bilayers of two materials with high scattering contrast, for example nickel and titanium.[7] The performance of a supermirror is usually characterized by its m-value, which specifies the resulting critical angle compared to natural nickel. For a complete description, the reflectivity as a function of incident angle has to be known. Some reflectivity files used for the simulations are shown in Figure 2.[8]

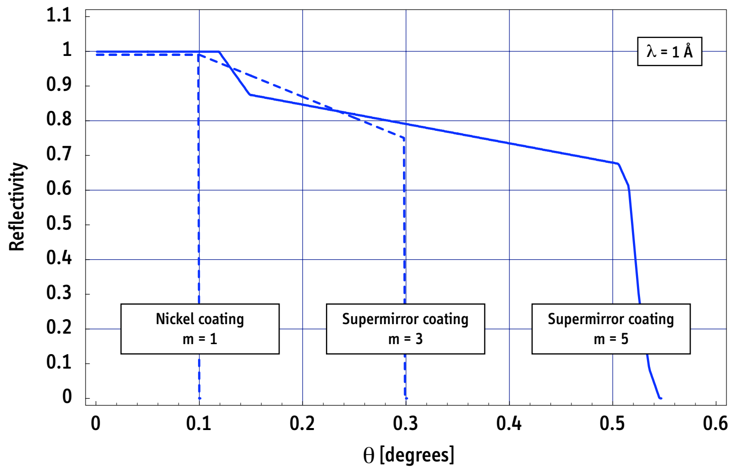

Figure 2: Reflectivity curves for neutrons at 1 Å used for VITESS simulations: natural nickel coating and supermirror coatings with m = 3 and m = 5. The curve for m = 5 has been fitted from experimental data for a coating produced by *SwissNeutronics*.[8] Other reflectivity curves are from the default data libraries.

To demonstrate the impact of supermirror technology, we model a standard guide with a square cross-section of 10×10 cm^2 and a length of 30 m, followed by a linearly tapered focussing guide of 5-meter length and an exit-width of 5×5 cm^2. A slight horizontal curvature with a radius of 2500 m avoids a direct view on the source and reduces the fast-neutron background at the exit and sample position.

The main results for this guide are shown in Figure 3. As expected, relative neutron intensities increase across all relevant wavelengths with increasing m-values. Compared to the standard nickel-coating, the most significant improvement is observed for m = 2. Higher m-values further improve the performance of the guide, but only for wavelengths below 4 Å. For example, at 2 Å, the guide with m = 3 yields a more than 3-fold increase in neutron intensity compared to m = 2. For wavelengths above 4 Å, neutrons are propagated without additional losses for all supermirrors, and little can be gained by using advanced coatings in this wavelength-band. Relative gain factors are shown in Figure 5 further below.

Elliptical Guide Geometry

Traditional neutron guides are characterized by rectangular cross-sections. The concept of the so-called ballistic guide was first introduced in the 1990s and recently developed further with the elliptical guide, which minimizes the total number of neutron-reflections along the flight path.[9] Here, we use a reference guide with entrance and exit dimensions of 10×10 cm^2 and 5×5 cm^2, respectively. The focal distances are about 200 cm in front of the entrance, i.e., very close to the neutron source, and 50 cm beyond the exit. The overall length of the guide is 35 m, its maximum width about 21.8 cm.

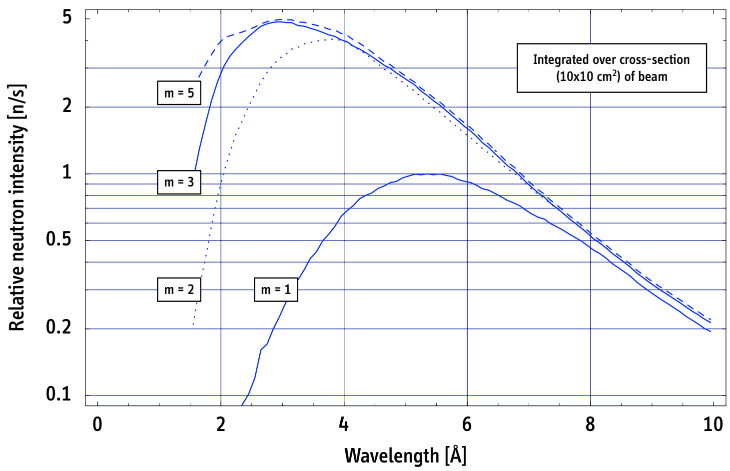

Figure 3: Relative neutron intensity $\phi(\lambda)\cdot A$ for the standard guide and various supermirror coatings (m = 2–5) relative to ordinary nickel coating. Intensity is integrated over the entire cross-section of the monitored beam.

As already visualized in Figure 1, one distinctive feature of the elliptical guide is the strong focussing of the neutrons compared to standard guides—usually an important advantage given typical sample sizes.[10] To account for this effect, neutron intensity is not averaged over the entire cross-section of the beam, as done previously, but integrated over the central region of the beam only.

Figure 4 shows the relative neutron intensity as a function of neutron wavelength. It compares a neutron guide with m = 2 and fixed cross-section, which is the standard today at modern facilities, with an elliptical guide using a supermirror coating of m = 3. In all cases, the gain in neutron intensity is taken at the distance with best focussing conditions: 75 cm for the standard and 50 cm for the elliptical guide.

Effective gain factors for selected combinations of coatings and geometries are shown in Figure 5. Most significantly, the elliptical guide delivers a gain factor of two for all wavelenghts above 5 Å, which is primarily due to the superior focussing characteristics of the guide. Compared to the standard guide, the gain is slightly smaller between 3–5 Å, but increases strongly for shorter wavelengths as a result of the higher m-value.

An important aspect of building high-performance but affordable elliptical guides is the possibility of using the highest m-material only near the entrance and the exit, where the curvature is strongest and most of the reflections occur. The m-value of the coating in the main section of the guide is far less relevant than in the case of standard guides. The performance of an elliptical guide for wavelengths below 6 Å can therefore be further increased, without significant additional cost. Specifically, using an advanced coating with m = 5 in an elliptical guide yields a two- to three-fold increase in neutron intensity between 3 Å and 4 Å, and a seven-fold increase at 2 Å compared to the standard guide with m = 2. This phenomenon, which is illustrated in Figure 5, opens up entirely new perspectives for neutron experiments in this wavelength range.

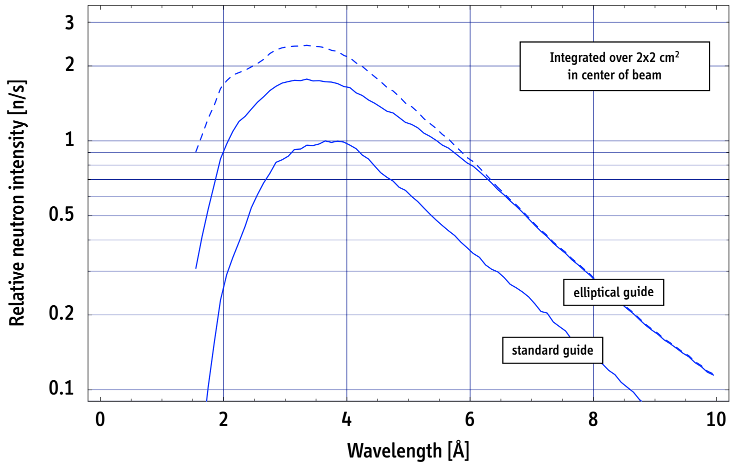

Figure 4: Relative neutron intensity $\phi(\lambda) \cdot A^{\star}$ for supermirror coating m $=$ 3 used in the elliptical guide relative to a standard guide with constant cross-section and m $=$ 2. Intensity is integrated over $A^{\star} = 2{\times}2$ cm^2 in the center of the beam and taken at the optimum distance from the guide exit. Results for an elliptical guide with m $=$ 5 (dashed line) are also shown.

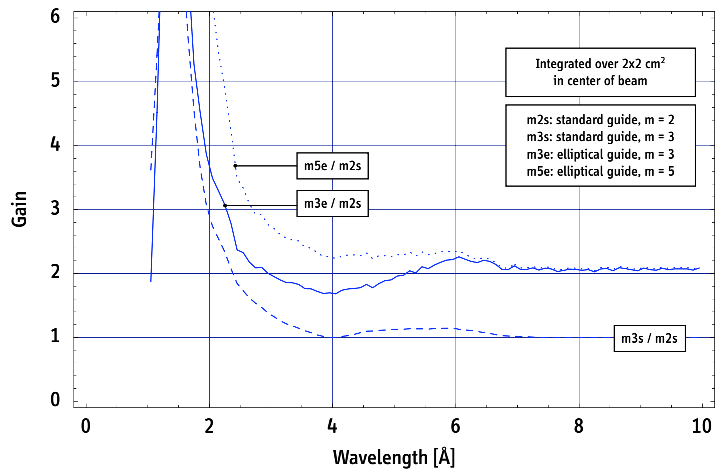

Figure 5: Neutron gain factors for various neutron-guide upgrade-options. Compared to the standard guide, the elliptical geometry delivers a gain factor of two for all wavelenghts above 5 Å, which is primarily due to the superior focussing characteristics of the guide. The gain is slightly smaller between 3–5 Å, but increases strongly for shorter wavelengths as a result of the higher m-value. Intensity is integrated over $A^{\star} = 2 \times 2$ cm^2 in the center of the beam and taken at the optimum distance from the guide exit.

Experience with Previous and Potential for Future Facility-Upgrades

The use of available neutrons for experiments at research reactors can be optimized with various strategies. The potential of advanced neutron-guide technology is of primary interest here, but other strategies include "quantitative" upgrades, in which the total number of instruments at a facility is increased. For example, between 1998 and 2006, six new scattering instruments at the High Flux Isotope Reactor (HFIR) in Oak Ridge have been added, bringing the total from 9 to 15 instruments with a corresponding increase in facility performance.[11]

Additional strategies for neutron-use optimization include renewal or upgrade of components and instruments. Virtually all elements of the experimental setup—from the cold neutron source, neutron guide, sample environment, and detector technology—may offer potential for improvement. In the case of the NBSR at the National Institute of Standards and Technology (NIST), for example, a two-fold increase in available neutron flux has been reported after replacement of the reactor's cold neutron source in 2002. A second replacement with a similar expected performance gain is now planned.[12]

The most comprehensive effort at upgrading performance is underway at the High-Flux Reactor (HFR) at ILL. Initiated in the year 2000, this so-called "Millennium Programme" envisions systematic modernization of the reactor's instruments and infrastructure. As illustrated in Figure 6, a sixteen-fold increase in overall performance of the facility is expected as a result of this ambitious long-term initiative.[13] A significant fraction of this gain is due to neutron-guide renewals alone.

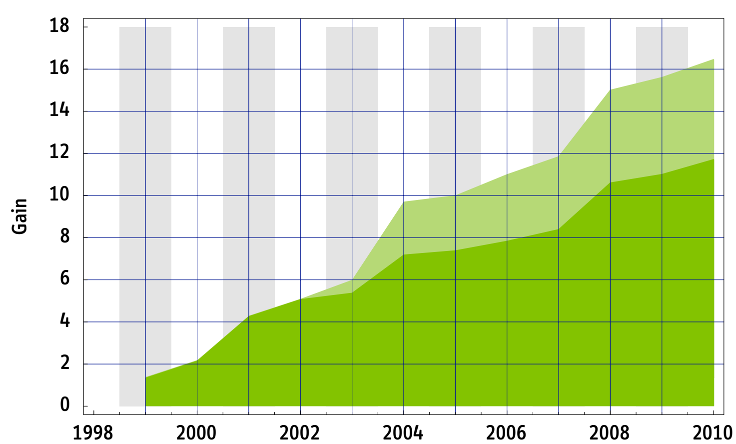

Figure 6: Performance gain of the High-Flux Reactor (HFR) at ILL. Contributions are due to instrument upgrades (dark-shaded area) and post-2002 guide renewals (light-shaded area).[13]

In general, the greatest performance gains can be expected for facilities where upgrades are most overdue. As of 2007, some neutron research facilities don't use supermirror coatings at all, very few facilities worldwide use coatings with $m > 2$ on their neutron guides, and virtually none use elliptical guides.[14] For example, the presently installed cold neutron guides of the FRM-II, which began routine operation as recently as 2005 at Munich University of Technology (TUM) and is currently HEU-fueled, typically use a coating of m = 2.[15] Thus, even the most modern facilities might be able to benefit significantly from more advanced neutron optics.

Funding has to be available to carry out such upgrades. The costs of conversion, operating costs, and the costs for upgrading neutron guides or instruments, however, are generally comparable to each other. *Investments in instrument-performance are therefore quickly recovered.* For example, less than $1 million is needed to install or replace a modern neutron guide.[16] This is a significant investment, but it has to be compared to the operating costs of a modern research reactor. Specifically, the costs of a typical high-flux-reactor fuel element are on the order of $1 to $1.5 million, and five to eight new fuel elements are needed each year. A two-fold increase in neutron flux at the experimental positions, and a respective increase of experiments that can be carried out at the facility, could pay off in less than two years—even if 10 neutron guides have to be replaced to achieve this overall performance gain.

Conclusion and Outlook

We have shown the tremendous potential of using supermirror coatings and elliptical guide geometries to optimize the neutron flux available for experiments at research facilities. The results of our simulations show that a *several-fold* increase in neutron intensity can generally be expected, even by upgrades to the neutron guides alone.

The performance gain from using a combination of advanced neutron-guide technologies has important implications for international efforts to end the use of highly enriched uranium fuel in research reactors. Converting these reactors to use low-enriched fuel often brings small losses in neutron flux. Our analysis demonstrates that the potential flux penalties due to conversion from HEU to LEU fuel become effectively irrelevant if a facility also upgrades its neutron guides.

Funding a program to simultaneously convert a research reactor to low-enriched fuel *and* upgrade its neutron guides need not be a significant constraint. The typical costs of conversion, operating costs, and the costs for upgrading neutron guides or instruments are generally comparable. Investments in instrument-performance are therefore quickly recovered. Given that there is now broad international support to end the use of highly enriched uranium in the civilian nuclear fuel cycle, and to establish regional centers of excellence for neutron research, it appears that the next few years may present research reactor operators and neutron instrument groups with a unique opportunity to coordinate a combined convert-and-upgrade strategy and achieve a significantly improved overall performance.

Endnotes

[1]High-flux reactors require about 500 kg out of the 1000 kg of HEU used in research reactors worldwide each year. 500 kg of HEU are sufficient to make 10–40 nuclear weapons.

[2]United Nations International Nuclear Fuel Cycle Evaluation (INFCE), *Report of INFCE Working Group 8: Advanced Fuel Cycle and Reactor Concepts,* Vienna, 1980, pp. 17–19, pp. 42–46, and pp. 137–172.

[3]Several journals publish articles on neutron-instrument optimization and related aspects, namely *Nuclear Instruments and Methods in Physics Research, Section A,* and *Physica B: Condensed Matter.* There is also a series of international conferences on neutron optics and instrument design using computer modeling. Among the more recent events are: the *European Workshop on Neutron Optics (NOP 2007),* March 5–7, 2007, Paul Scherrer Institute (PSI), Switzerland, kur.web.psi.ch; and the *International Workshop on Applications of Advanced Monte Carlo Simulations in Neutron Scattering,* October, 2–4, 2006, PSI, Switzerland, lns00.psi.ch/mcworkshop.

[4]Besides VITESS, several other dedicated Monte Carlo computer codes simulate propagation of neutrons through complex instrument architectures (for example, McStas and RESTRAX). VITESS Release 2.6 has been used for all simulations presented here. See www.hmi.de/projects/ess/vitess for more information and updates.

[5]The code follows a modular approach, in which individual modules are connected in series and pass neutron-data through the modeled system. Available modules include several types of neutron sources, neutron guides, choppers, monochromators, samples, etc. In addition, dedicated modules are available to monitor the neutron-beam, which is characterized by 12 coordinates, at arbitrary positions along the beam. Instruments that can be modeled in VITESS include crystal analyzer backscattering spectrometers, small angle neutron scattering (SANS) instruments, neutron spin echo spectrometers, powder diffractometers, and reflectometers. Time-of-flight modes can be simulated, if applicable.

[6]This is a typical value. In general, it is preferable to move the guide entrance closer to the (cold) neutron source, but this strategy is limited by strongly increasing irradiation damage to the guide entrance and other constraints.

[7]For a discussion of the underlying physics and design principles, see C. Rehm, M. Agamalian, F. Klose, *Neutron Supermirrors: Design and Application,* Report of the Optical Components Team, Spallation Neutron Source Project, Oak Ridge National Laboratory, May 2002.

[8]Shown reflectivity files are mirr1a.dat and mirr30std.dat for m = 1 and m = 3, respectively. Additional results for m = 2 are based on mirr2linear.dat (not shown). Data for the advanced supermirror coating fitted from experimental data provided by *SwissNeutronics*, private communication, May 2007.

[9]C. Schanzer, P. Böni, U. Filges, and T. Hils, "Advanced geometries for ballistic neutron guides," *Nuclear Instruments and Methods in Physics Research, Section A,* 529 (2004), pp. 63–68.

[10]The divergence of the neutron beam increases in this situation, which is is unfavorable for certain types of experiments and instruments, in particular for Small-Angle Neutron Scattering (SANS).

[11]Information on HFIR instrument systems is available at neutrons.ornl.gov.

[12]See NIST Center for Neutron Research, *Annual Report 2002,* National Institute of Standards and Technology, pp. 6–7 and *Annual Report 2006,* p. 50. For more information, visit www.ncnr.nist.gov.

[13]D. Dubbers, "The Institute Laue-Langevin and its Role in Neutron Science," Presentation at the ILL Millennium Symposium and European User Meeting, Grenoble, April 27–29, 2006. Data for expected performance gain taken from Slide 19. In 2006, the budget of the program was about 6 million Euro for both instruments and infrastructure. In total, about 30 million Euro had been expended by then, which corresponds to about half of the total expected costs. For more details on this initiative, see R. Wagner, "ILL Millennium Programme: Achievements for the benefit of ILL's user community," presentation at the same meeting.

[14]As of 2007, not a single neutron research facility is using even one fully elliptical guide, as modeled and discussed above. A 1:10 scale model is studied at the spallation neutron source SINQ at PSI in Switzerland, where a first elliptical guide might be installed by 2010. The first facility to use full-scale elliptical-guide technology could be ISIS in the United Kingdom.

[15]K. Zeitelhack et al., "Measurement of neutron flux and beam divergence at the cold neutron guide system of the new Munich research reactor FRM-II," *Nuclear Instruments and Methods in Physics Research A,* 560 (2006), pp. 444–463.

[16]See Rehm et al., *op. cit.*, for a breakdown of relevant costs.