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Global guide study for cold and thermal guides Ladi3@H112 guide simulation: effect of a double curved guide

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Abstract

We have been looking in this report at ILL sources, available capture flux measurements and simulation results using *McStas*.

The measurements show that most existing guides behave as they should, even though a significant (30 %) loss has been observed since they were installed. But some particular guides (H142, H511, H22, H53, and to a lower extent H18, and H21) seem to show unexpected flux loss. More specific measurements are required in order to determine if the flux loss is indeed abnormal, or it results from characterized effects (alignment, monochromator diffraction/scattering, uncertainty on the determination of measurement position, additional optics, *etc*). The flux simulations (on the basis of the available information) show that these guides should not present such losses .

The HCS source provides more neutrons than what is expected from published source characteristics data. On the other hand, the thermal ambient flux model in the core seems lower than the published value. The VCS source modelling gives absolute flux values very close to the observed data. Some MCNP/Tripoli computations would be required to possibly achieve a better accuracy in the spectral description of the sources.

From this study we may propose a list of actions:

Priority 1

- Gold foil campaign on ILL guides, particularly H141, H142, H53, H512 and H511.
- Check of the H511 guide
- Check of the H142 second curved section.
- Check of the H53 last 10 m section.
- Check/Update of capture flux distances from moderator/reactor. Use GPS/Laser positioning.

Priority 2

- Compute ILL HFR reactor models for the HCS, VCS and thermal spectrum (from Tripoli/MCNP)
- Check/Update of instrument distances from moderator/reactor. Use GPS/Laser positioning.

The construction of new guides such as H112 may be envisaged once the anomalous flux losses have been investigated and understood. A simulation of such a double-curved guide for LADI3 has been performed, showing that focusing of the beam is a natural consequence of the curvature and could therefore be tuned to instrument requirements. Significant flux gains would be achieved compared to the present H142 position, with a limited effect on the divergence.

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This study is the result of a 3 years investment, most of the time under the request of the DS and the DPT. The level of accuracy in the description of guides and sources characteristics, as well as the overall understanding of neutron beam phenomena taking place in guides and at the instrument positions has continuously been improved.

This report is, to my knowledge, the first cross-comparison of neutron capture flux measurements as a function of distances for most ILL guides and sources, together with accurate guide simulations.

In the course of this study we focused on the ILL source data, the geometry of guides, and the available flux measurements. Simulation results are in agreement with most neutron capture flux measurements, except for a few identified guides which reveal anomalous flux losses.

Some of the H112 results which give relevant additional information on the neutron beam at the end of guides (sections G and H) have also been presented in a previous report [17].

A - About the ILL HFR reactor and moderators

The sources used to produce neutron particles in the simulation is a volume that illuminates the guide input window with a given spectrum. For the following results, this spectrum is modelled as three Maxwellians fitting reference flux data.

Concerning the cold moderators, the calibration data was obtained using Tripoli and MCNP [1]. Additionally, the HCS spectrum was indirectly measured in [1]. When plotting all the existing cold sources data (see *Figure 1*), we notice significant differences for the HCS, not only between indirectly measured and calculated data, but even between the two available 'calculated' models. One of these models may take into account absorption effects in the beam tubes. Anyway, according to the *Figure 1*, the expected HCS flux in the cold neutron range is not significantly different from the VCS one. Whatever the chosen model , if we use this raw data, the simulated capture fluxes for cold guides using the HCS model are lower than the measured ones, whereas this is not the case for the VCS. This would mean that the published HCS spectrum data is underestimated (by a factor 2).

On the other hand, the Thermal spectrum is extracted from the ILL Yellow Book, 1988 edition using the H12 beam tube data [2]. The simulated capture flux for thermal guide are then higher than the measured one (by a factor 2.25), assuming a thermal unperturbed flux.

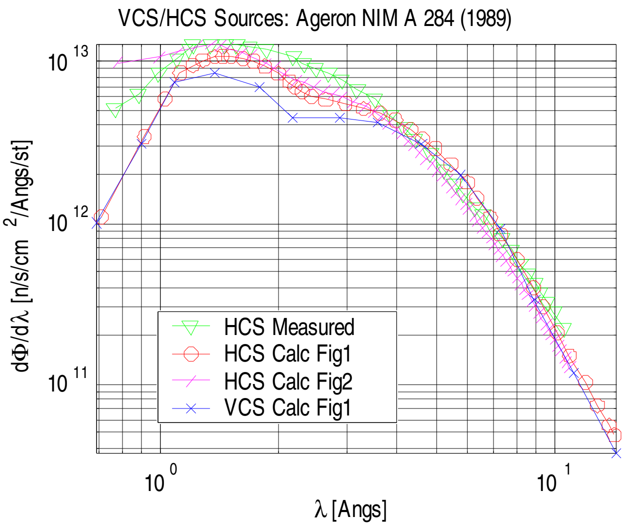

Figure 1: Source spectra extracted from [1]. VCS model gives accurate simulated results, but the HCS model gives lower fluxes than measured ones. The 'HCS Measured' model (extracted from Fig 2 of [1]) gives about the same cold neutron flux as the two 'HCS Calculated' models in the λ =4-10 Å range.

We did not look at the hot source beam tubes in this study.

In a few words, if we use the published data for the source models [1,2], all the simulations that I could perform are in agreement with measurements within a factor 2 (see *Table 1*). We shall see that only a few neutron guides show unexpected characteristics.

For all the following results, we have multiplied the HCS flux from [1] by a factor 2, whereas we have divided the Thermal flux from the H12 beam tube [2] by a factor 2.25, in order to compare directly simulated and measured capture fluxes.

Source/Moderator	***Notes concerning published data [1,2]***
VCS (H1x, IH1)	Provides simulated flux *in agreement* with measurements within a few percent
HCS (H5)	Provides simulated flux *lower* than measurements by a factor 2
Thermal (H2x, IH3, H6-7, H9-13)	Provides simulated flux *higher* than measurements by a factor 2.25
Hot (H3, H4, H8)	Not simulated

Table 1: Comments on the ILL reactor and moderators with discrepancy ratio required to cope with measurement data (capture fluxes) using published spectrum data and *McStas* models.

B - Comment on the absolute capture fluxes

The available ILL flux data for guides and instruments may be classified into two sets.

The gold foil capture fluxes are obtained from a standard procedure, unchanged from the ILL early days. Measurements have been achieved on a regular basis, and at quite a number of locations along the guides. The only uncertainty resides in the history of guides/instruments (which I do not know anything about), and for some particular cases, in the measurement conditions (was there a filter ? Was the beam polarized ? Was the tube under atmospheric pressure ? Is the distance to the reactor well known ? Reactor power ?). The data from Kaiser, Gahler and Bazzoli [3] shows that an average 30 % flux loss has been observed for all ILL guides since 1980. As a complement, we have plotted (see *Figures 3-6* further in this report) these data as a function of the distance from the measurement position to the reactor. The accuracy of these capture fluxes is estimated to be within 10 %. The distances from the core for these measurements, indicated in [3], do not correspond with existing gaps (according to drawings [6-11]) where the measurement could be achieved. We thus believe that errors as large as 5-10 meters may exist on the measurement position, which have an effect on the loss per meter curves (see *Figure 3-6*). For some guide, H141, H512, there is currently no capture flux data available.

All the capture flux measurements used in this paper are the highest reported values for each guide (usually just after commissioning), so that the guides are as ideal as possible, in order to be compared with the simulation model which describes a perfect situation. The present values are lower, due to guide damage and misalignment.

At instruments positions, the flux *vs.* wavelength λ curves are usually available. Unfortunately, these measurements depend intrinsically on the monochromatisation device (chopper, monochromator, velocity selector). Each measurement point is indeed the integral of the incoming flux on the transmission window, which spectral shape is very specific to each device. Thus, even if the instrument scientists do compare fluxes and their evolution with time for each instrument, we can not use this data as a global, absolute measurement of fluxes for comparison between guides and sources.

In this study, most of the time, we have extracted a white beam from the source/moderator, and illuminated monitors positioned along guides. These monitors have been set to measure the integral:

$$\Phi_c = \int \frac{\lambda}{\lambda_0} \frac{\mathbf{d}\Phi}{\mathbf{d}\lambda} \mathbf{d}\lambda \quad [\mathrm{n/s/cm^2}] \text{ with } \lambda_0 = 1.8\ \text{Å}.$$

Additionally, absolute flux curves *vs.* wavelength have been extracted.

C - Guide geometry and characteristics

All guide models have been built using the ILL drawings [4-11] as well as some 'raw' specification sheets as in Ref. [3]. A special care was given to the description of the elements along the guides, including gaps (between elements, sections and around monochromators), and aluminium windows. The loss mechanisms that may take place within guides have been studied in previous reports, as well as in [16].

Guides are described as a set of sections of elements, for which reflectivity is modelled as an analytic function. The reflectivity model values are extracted from fits performed using reference measured reflectivity curves from I. Anderson and K. Andersen. In the model, the guides are perfectly aligned, reflectivity and glass quality are constant .

As an example of such a guide model, we now focus on the H112 guide project [8]. Other simulations are quite close, except for the source, curvature radius, length, gaps and number of elements.

D - Example: The H112 Guide description

The H112 guide project is still under design process. Anyway, the geometrical constrains are quite strong, as it has to fit in the middle of the H22 and H23 thermal guides, and be bent enough to come at a usable upper plane (say 1 meter up).

Today, the envisaged upper channel geometry is a double bent guide (1.5 km horizontally, 2 km vertically), made of 1 meter elements, along about 80 meters [8]. The coating would be full m=2 super mirror (including *in-pile* part). Section would be 12h x 6w (in cm^2), split into 3h x 6w and 8h x 6w after 30 meters. The lower channel geometry is still to be defined, but would only have an horizontal curvature.

The simulated guide model contains the elements listed in *Table 2.* Aluminium windows and gaps are in the model. The coating is assumed to produce a SM92 reflectivity curve (given by the mean value in the decreasing sloppy region, with $R_{m=1}$=0.99 and $R_{m=2}$=0.84). Actually, super mirrors in production today may reach much better specifications ($R_{m=2}$=0.92), which would bring even more flux than the current simulation results. Anyway, using a lower reflectivity is a way to take into account imperfections such as the guide misalignment, the coating and substrate inhomogeneities, the waviness, etc. Some of these effects are not explicitly in the guide element model we have used.

The HCS and VCS specifications are taken from [1], and multiplied by a factor 2 for the former. The *Figure 1* shows a view of the model. The guide alignment is considered to be perfect.

Element	***Detail of model***	***Specifications***
Source	Vertical Cold Source [1]	22h x 14w [cm^2]
Pink Carter	Focusing, m=2 coating	w=68->60 mm, h=12 cm, L=3.17 m
Lead Shutter	m=2	L=0.228 m
H112-2	Polygonal, 6 elements, m=2	L=6.1 m, w=60 mm, h=120 mm, r=1.5 km
Vacuum space	For the V.S.	L=0.2 m
H112-3, H112-4, H112-5	Polygonal, 20 elements, m=2	L= 20.5 m, w=60 mm, h=120 mm, r_h=1.5 km, r_v=2.0 km
Vacuum space	For the V.T.E. Guide splitting	L=0.33 m
H112-6, H112-7, H112-8, H112-9, H112-10	Polygonal, 50 elements, m=2	L=50 m, w=60 mm, h=30 mm, r_h=1.5 km, r_v=2.0 km

Element	*Detail of model*	*Specifications*
End of guide: Ladi3 position	(Sample is at 3 m)	

Table 2: H112 guide geometry [8].

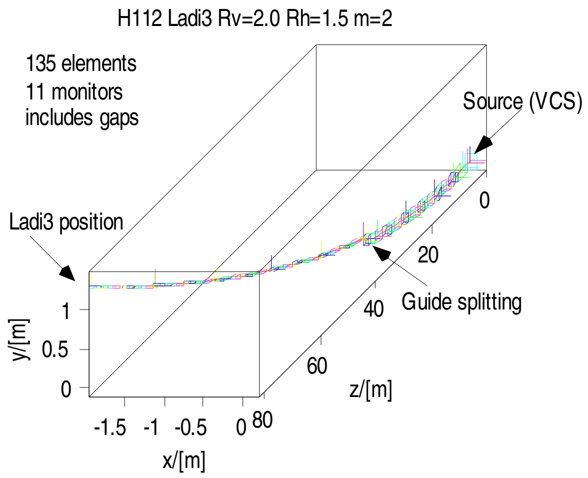

Figure 2: Geometric view of the H112 guide model, as seen from the IN12 side of ILL7 building.

The simulation package is *McStas* [13] version 1.8. Similar simulations where carried out in 2001, and are reported in [14,15].

E - Scope of this study

We have chosen to study a representative set of ILL guides, using the same procedure for all simulations, so that absolute guide comparison can be achieved.

Guide	*Measured*	*Measured* **and** *Simulated*
Cold 'classical' ILL7	H16, H17, H18	H142, H15
Cold 'improved' ILL7		H113, *H112 as a project*
Cold ILL22	H511, H512	H53
Thermal ILL7	H21, H22, H23, H25	H24

Table 3: Scope of this study

Anomalous guide	*What's wrong with it*
H142	Flux loss after the VTE (30 m from core)
H53	Flux loss in the last 10 meters
H511 (polarized)	Flux loss all along. *Not simulated.*
H22	Flux loss in the last 20 meters. *Not simulated* but H24 (similar geometry) was simulated.

Table 4: Anomalous guides (from measured capture flux data)

Looking at the measured capture flux data, it is clear that guides may be sorted into classes according to flux variation as a function of time (since 1972) and location (distance from the core). The *Table 3* defines these classes. Moreover, without any simulation results in mind, some guides seem to have 'strange' behaviour (see *Figures 3-6*). These particular guides are listed in *Table 4*.

F - Simulated neutron capture fluxes

We present in *Figures 3-6* both the measured capture fluxes, as a function of the distance to the core, taken from the commissioning data of Ref. [3], and the simulated capture fluxes for a selection of representative guides (see *Table 3*, right column). No optics were positioned in the simulated guides, but the associated gaps (*e.g.* around monochromators) are definitely in the models.

Legends indicate the guide label, as well as its curvature radius *R* in km, its coating *m*-value, and its section in cm^2. The open symbols are capture flux gold foil measurements, whereas full symbols are simulation results (labelled as ' simàs well).

1 - ILL 22 Cold guides (H5)

The H511 guide was not simulated, as polarized neutron guides introduce additional complexity in simulations. The H512 guide, according to the single available capture flux measurement, behaves the same as H53. This latter shows (see Figure 3) an important flux drop in the last 10 meters. According to the simulation results, this drop is essentially given by the numerous monochromators in beam, which both diffract a significant part of the flux and possibly scatter an other part on the mechanics (SANS, incoherent). Indeed, in the simulation, only the gaps around the monochromator positions have been accounted for, resulting in a more limited flux drop. A simple test for this would be to bring all monochromators to a non useful position (short wavelength) for the gold foil measurements downstream. As explained in section A, the ILL22 simulations uses the HCS 'Measured' data from [1] multiplied by a factor 2 in order to fit the measured capture fluxes.

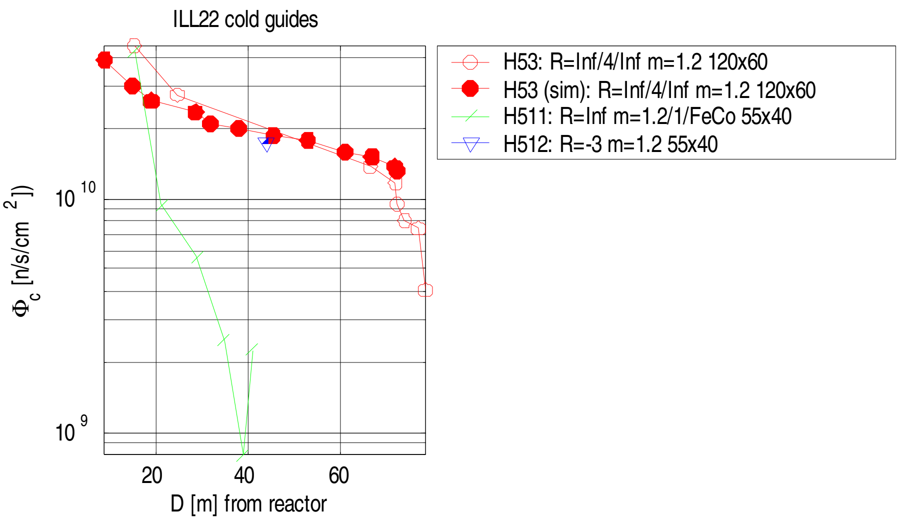

Figure 3: The ILL 22 Cold guides (H5) capture flux measurements (open symbols) and simulated H53 (•).

For these guides, we recommend to have a close look at the H511 guide, and at the end of H53. More measurements on H512 are required.

2 - ILL 7 Classical cold guides (H1)

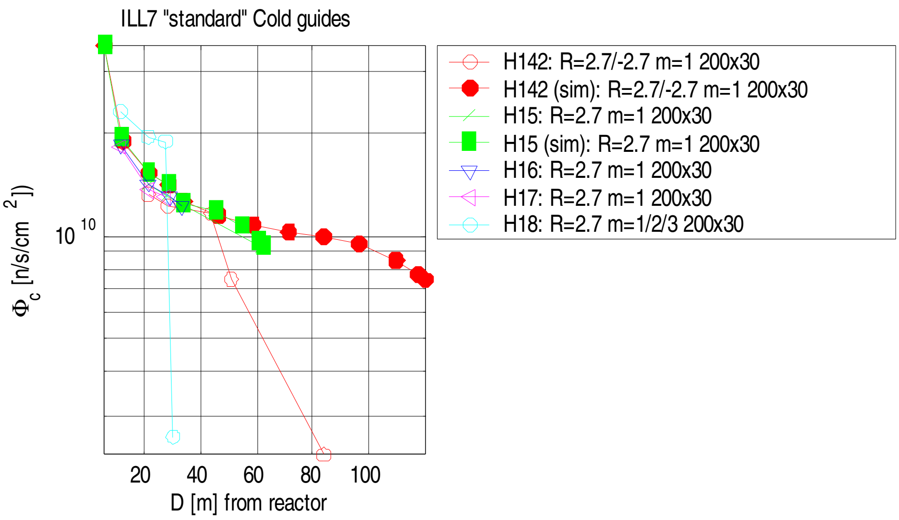

Figure 4: The ILL7 Cold guides (H1) capture flux measurements (open symbols) and simulated H15 (■) and H142 (•).

All the Nickel guides from ILL 7 bring the same flux to the instruments, except H142 and H18 (see *Figure 4*). The former shows a kink in the losses while the latter shows a drop at the end, which is probably associated with the focusing funnel. The simulated H142 follows the same behaviour as the other guides. Then, either the second curved section (H142 is an *S*-guide) is damaged, or the distance from the core for the capture flux measurements is wrong (see comment on this in section *B*). Also, the in-beam monochromators (IN12, T3) possibly diffract/scatter a significant portion of the spectra. A simple test for this would be to bring it to a non useful position (small wavelength) for the gold foil measurements downstream.
The VCS moderator data [1] produces absolute flux in excellent agreement with measurements without any correction.

For these guides, we recommend to have a look at the H142 (and possibly H18) guide.

3 - ILL 7 Improved cold guides (H1)

The super-mirror guide H113 is the closest existing guide comparable with the H112 project. We show (see *Figure 5*) that absolute fluxes, including the ballistic effect (focusing at the end of the guide), may be simulated without any correction.
Similar flux values will be obtained with the H112 super-mirror guide, even though the H112 upper channel project is a double bent guide, and thus suffers from additional losses (more reflections on the sides) compared with an ILL guide as H15. This is clearly visible for the ' H12 m=1' classical guide simulation (compare with *Figure 4, H15* ■). This means that a horizontal classical super-mirror guide as the H112 horizontal lower channel (see section D) will probably benefit from a higher flux as H113.

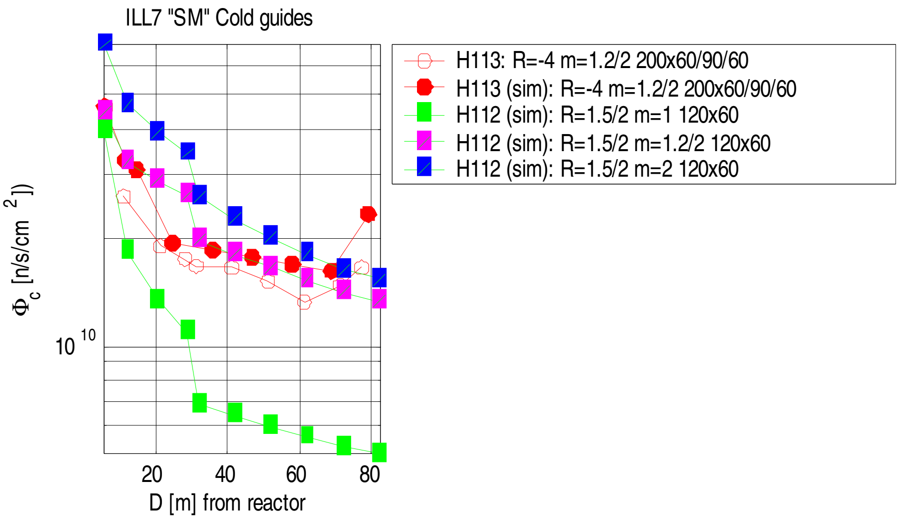

Figure 5: The ILL7 ' improved' Cold guides (H1) capture flux measurements (**o**) and simulated H112 (■■■) and H113 (•).

4 - ILL 7 Thermal guides (H2)

All the ILL7 Thermal guides follow the same behaviour, even though their curvature radius differs significantly, but the H21 and H22 guides show some additional flux losses in the last guide sections. As stated for the other cold guides, this may be the result of instrument monochromators extracting (diffraction/scattering) significant portions of the spectra. New capture flux measurements with un-tuned monochromators would probably be required.

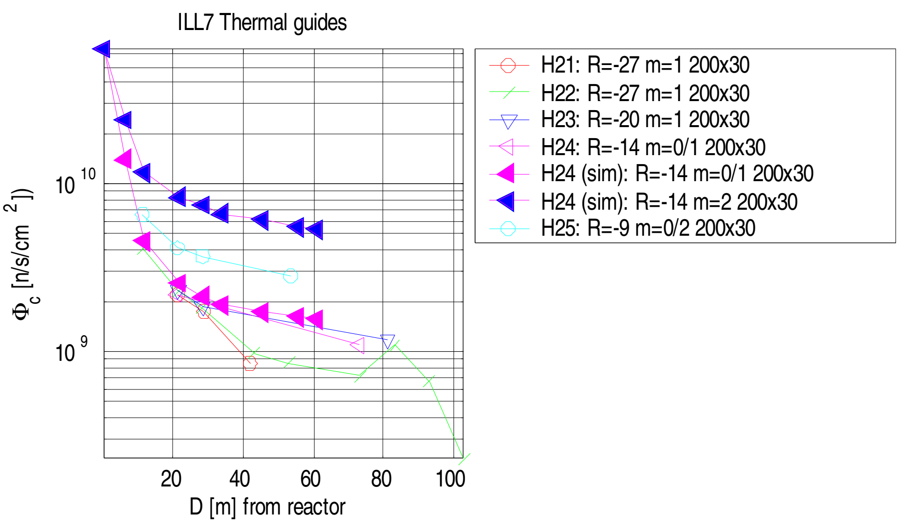

Figure 6: The ILL7 Thermal guides (H2) capture flux measurements (open symbols) and simulated H24 (filled triangles).

We simulated the H24 guide (see *Figure 6*) in present as well as in full super-mirror configurations. The H25 super-mirror guide, with classical in-pile part, fits in between. According to this study, the fully super-mirror coated thermal guide would bring about a factor 3 gain in capture flux compared to present values.

As explained in section *A*, the ILL7 thermal simulations uses the Yellow Book H12 data from [2] divided by a factor 2.25 in order to fit the measured capture fluxes.

G – Flux at the end of guides

We present in *Table 5* the measured and simulated capture fluxes at the end of some ILL neutron guides. The measured values are obtained from [3], with an uncertainty for measurement position (distances from the core) which appears when comparing the values with the drawings from the Bureau d' Etude [4-11]. The measured capture flux are within 10 %, and the simulation accuracy is estimated to be below 5 %.

Guide	***Φ_c [n/s/cm2] simulated***	***Φ_c [n/s/cm2] (Meas. gold foil)***	***Comment***
H112 Rh=1.5 Rv=0 km m=2	**17.0 10^9**		**In-plane project (lower channel)**
H112 Rh=1.5 Rv=2 km m=1.2/2	**13.4 10^9**		
H112 Rh=1.5 Rv=2 km m=2	**15.3 10^9**		***In-pile* part upgraded**
H113 (PF1b) Rh=4 km m=2	**30.1 10^9**		***In-pile* part upgraded**
H113 (PF1b) Rh=4 km m=1.2/2	23.4 10^9	16.5 10^9 (in 2000, at z=77.4 m)	Ballistic 6/9/6 cm
H15 Rh=2.7 km m=1 *(H16 -17 are similar)*	9.3 10^9	9.3 10^9 (in 1972 at z=61.2 m)	Similar as H16 and H17 but lengths are different
H142 Rh=2.7/-2.7 m=1 (LADI)	7.4 10^9	2.1 10^9, **losses starting at splitting pos.**	S-curved
H53 Rh=4 km m=1.2	16.2 10^9	11.6 10^9 (in 1988 at z=72 m)	HCS Calculated [1] times 2
H53 Rh=4 km m=1.2	13.2 10^9	***Factor 3 loss after IN16***	HCS ' Measured' [1] times 2
H511 m=1.2/1/FeCo	*Not simulated*	1-2 10^9 (in 1996 at IN15)	**High losses (factor 10 *w/r* to H53)**
H512 Rh=3 km m=1.2	*Not simulated*	17.4 10^9 (in 1988 at z=38 m)	In agreement with H53
H24 Rh=14 km m=0/1	1.7 10^9	1.28 10^9 (in 1985 at z=73 m)	H12 beam tube [2] divided by 2.25
H24 Rh=14 km m=2	**5.5 10^9**	2.0 10^9 (on H25 in 1997 at z=73 m)	In-pile part *m* value meas.=0, **sim=2**

Table 5: Flux estimates for some ILL guides (end position). Horizontal *Rh* and vertical *Rv* curvature radius, and coating *m* value are indicated.

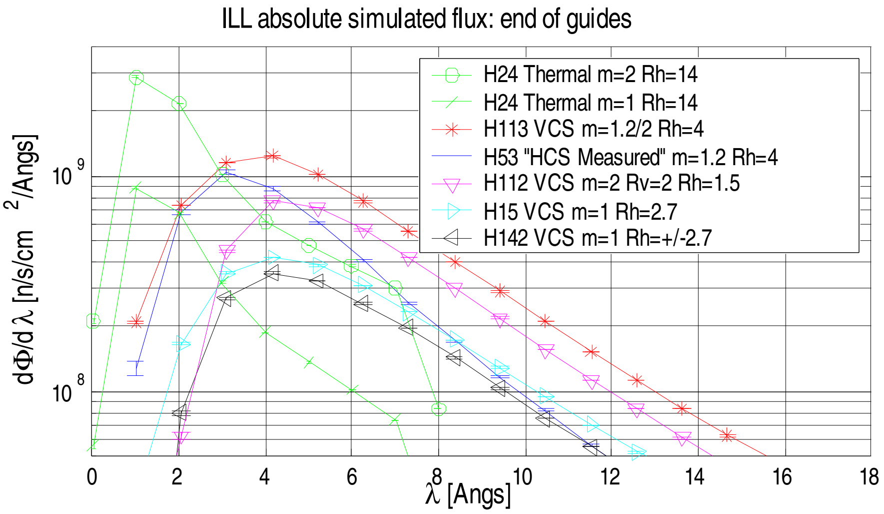

Figure 7: Simulated flux as a function of the wavelength for a set of guide end positions. The vertical R_v and horizontal R_h guide curvature, as well as the coating *m* are indicated.

As a complement, we have plotted the absolute simulated flux wavelength distribution at some guide end positions (*Figure 7*). The spectral shape is determined by the source spectra and the guide transmission, which essentially depends on the curvature and guide coating.

H - Simulated spatial and divergence distributions

In order to estimate the beam distributions at the H112 upper channel end of guide (LADI instrument), we have positioned monitors just at the end of the guide. The instrument sample position itself should come after a 3 m beam tube, with filters, slits and shields.

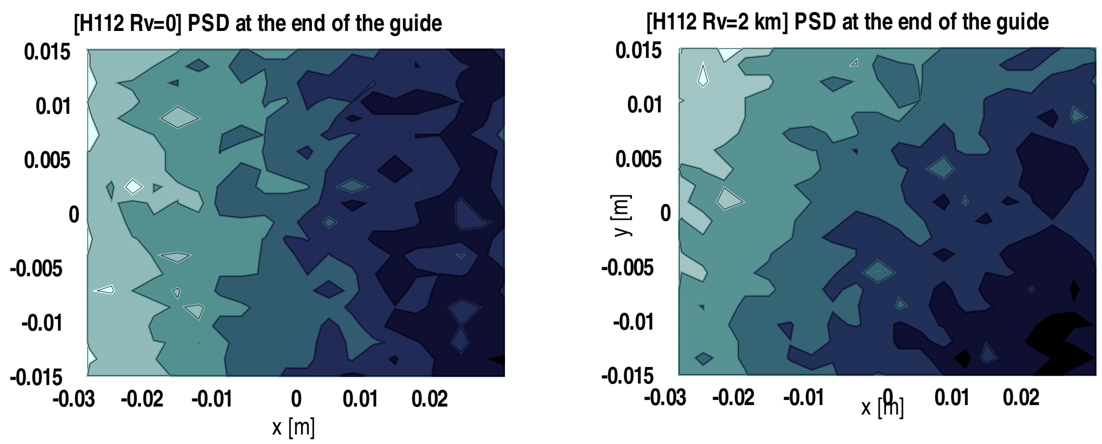

Figure 8: Neutron beam spatial distribution (PSD) at the exit of the H112 curved guide, at λ =5 Å. For both plots, the horizontal curvature is R_h=1.5 km. The plot on the right has an additional R_v=2 km vertical curvature. Dimensions are in meters. Intensity scale goes from the white (low) to black (high). Coating is *m*=2.

The analytical models [15] for curved guides do predict a shift of the beam after a curved guide. This shift is removed when adding a long enough straight section downstream. Looking at *Figure 8 – left plot*, this effect is indeed observed as expected: the beam intensity on the outer curvature side is 70 % higher than that of the inner side.

In the case of a horizontal and vertical curved guide, the shift occurs in both directions as presented in *Figure 8 – right plot*, and finally the beam is gathered in one corner of the guide, producing a natural focusing which might be of great interest for Laue diffractometers such as LADI. The ratio of the maximum to the minimum intensity in the guide section is about 2. Other instruments such as horizontal reflectometers may also benefit from vertically curved guide which would produce well defined pre-focussed horizontal beams.

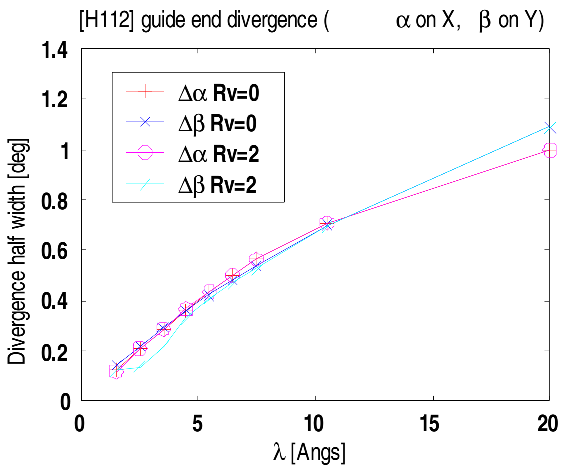

Figure 9: Neutron beam divergence half width Δα (on X) and Δβ (on Y) at the end of H112 as a function of the wavelength at the end of the H112 guide, with a vertical curvature R_v of 0 and 2 km. Coating is *m*=2.

The divergence (see *Figure 9*) is close to the well known linear law for long guides. The vertical curvature has a small effect on the vertical divergence, which is lowered at small wavelengths (for $\lambda < 5$ Å). A Nickel coated guide would have a lower divergence (by a factor 1.5). The divergence distribution at the end of the guide is not homogeneous: the highest intensity spots in *Figure 8* also have higher divergence.

In order to estimate the effect of the gravitation at the end of the H112 guide, at 80 meters from the moderator, we have plotted on *Figure 10* the ratio of the top over the bottom intensity extracted from the PSD projection on the vertical axis. When the vertical curvature R_v is zero (in-plane), the anisotropy becomes sensible only for $\lambda > 7$-10 Å. For 20 Å cold neutrons, the gravitation stacks about 14 % more flux on the bottom part than on the upper part of the beam.

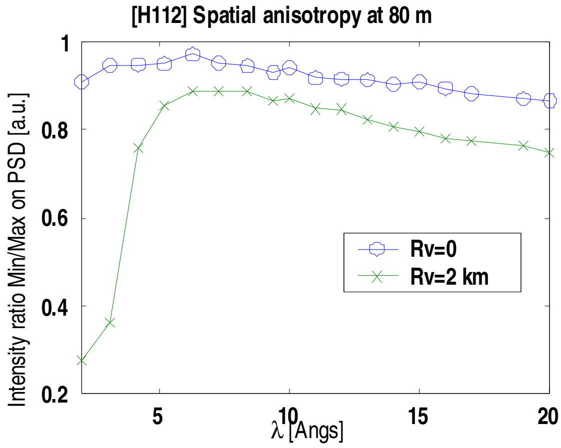

Figure 10: Gravitation effect: spatial vertical anisotropy measured as the ratio of the top over the bottom intensity of the projection of the PSD over the vertical axis, at the end of the H112 guide with R_h=1.5 km, R_v=0 and 2 km, *m*=2.

Concerning the H112 model with vertical curvature, the effects are more pronounced. For low wavelengths, only 'garland' reflections may occur in the guide [15], and the neutrons are stacked to the lower part. Then, reaching the guide critical wavelength (which is around 1.9 Å), the anisotropy is optimal (with still 10 % more neutrons on the bottom part), and becomes slowly worse for cold neutrons, reaching 25 % vertical anisotropy. This anisotropy will control the size and position of the slits for optimal beam flux.

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