Chapter 5

Instruments and Scientific Utilisation

Authors and Contributors

Instruments and Scientific Utilisation

Authors:

F Mezei,[1] R Eccleston,[2] H Tietze-Jaensch[3]

Contributors :

H Abele,[4] P Allenspach,[5] K Andersen,[2] A M Balagurov, [6] R Bewley,[2] H-J Bleif,[1] H Boerner,[7] H Bordallo,[1] J Rodriguez Carvajal,[8] D Colognesi,[2] B Cubitt,[7] R Cywinski,[9] M Daum,[5] M Daymond,[2] R Eccleston,[2] G Ehlers,[7] B Fak,[2] B Farago,[7] C Fermon,[8] H Fritzsche,[1] T Gutberlet,[1] R Heenan,[2] W Heil,[9] S Hull,[2] W Jauch,[1] O Kirstein,[10] R Lechner,[1] K Lefmann,[11] E Lehmann,[5] K Lieutenant,[1] T Lorentzen,[11] R McGreevy,[2] G McIntyre,[7] F Mezei,[1] M Monkenbusch,[10] K Mortensen,[11] H Mutka,[7] D Myles,[12] C Pappas,[1] J Peters,[1] P Radaelli,[2] H Rauch,[13] W Reimers,[1] H Ronnow,[7] B Schillinger,[14] D Schwahn,[10] W Schweika,[10] A Serebrov,[15] G Simpson,[7] A Soper,[2] A Steuwer,[16] R Stewart,[7] E Suard,[7] H Tietze-Jaensch,[3] J Webster,[2] A Wiedenmann,[1] C Wilson,[2] P Withers, [16] M Zoppi,[17] G Zsigmond[1]

[1]HMI Berlin, [2]ISIS, [3]ESS-CPT/FZJ, [4]Heidelberg, [5]PSI, [6]JINR, [7]ILL, [8]LLB, [9]Leeds, [10]FZJ, [11]Risø, [12]EMBL, [13]AI Wien, [14]TUM, [15]PNPI, [16]Manchester, [17]CNR

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Instruments and Scientific Utilisation

5 INSTRUMENTS AND SCIENTIFIC UTILISATION

5.1 OVERVIEW

The instruments are used to transform neutron scattering events into data from which scientific conclusions can be drawn. Thus defining and optimizing the instrument suite determines the scientific profile and potential of the whole facility. ESS is a science driven facility and hence the ESS Science Advisory Committee (SAC) and the Instrumentation Task Group (ITG) worked out the major parameters for ESS in close collaboration. Several joint workshops were held to arrive at a proposal for the number of and characteristics of the target stations, pulse characteristics and repetition rates etc. [Mezei, 2001], [Richter, 2001]. Moreover, ITG and SAC worked out and agreed upon the proposed generic instrument suite and defined priorities for the list of instruments. It was at the Engelberg workshop in May 2001 that the Long Pulse Target Station (LPTS) - a unique feature world-wide – replaced the 10 Hz SP target station in the ESS reference design. Shortly after May 2001 a number of instruments and instrumentation ideas for LPTS emerged and were simulated. Moreover, the new LPTS design called for a revision of both moderator concepts and neutron beam optics. Many of these initial ideas on instrumentation of the two complementary LP and SP target stations were presented at the ESS Conference in Bonn in May 2002 and the ESS documentation hitherto [ESS 2002, ESS 2002a]. More detailed work was presented at the ICANS XVI meeting in April 2003 in Neuss [Mank, 2003], [Mezei, 2003], [Tietze, 2003]. An evaluation of the ESS proposals on instrumentation and moderator concepts compared to SNS, JSNS and existing and planned European facilities was undertaken by the SAC and the ESFRI working group on neutrons [ESFRI, 2003]. Both the prospects of the LPTS and the possibility that a staged approach starting with the LPTS, might have a greater chance of being funded led the ESS-SAC in its last meeting to among others make the following recommendation: "The SAC suggests to focus attention to a staged approach for ESS taking into account the affordability and the scientific capabilities (road map). It is absolutely necessary to avoid compromises that could hamper the overall goal of a competitive source of highest performance." In this chapter we have therefore elaborated slightly on a staged approach also by investigating an optimised LP first stage by up-grading the power. Furthermore, we shall concentrate entirely on progress and novelties that were not fully documented previously.

Time between the Engelberg workshop and the Bonn conference was too short to produce a comprehensive Monte Carlo simulation of the revised moderator performance. Detailed MC results on pulse shapes, spectral properties and overall intensity of a technically feasible and optimized moderator/reflector layout is now available (cf. chap. 4, namely 4.1 of this report).

The next natural step in the ESS target-instrument-interface process would be to evaluate the results of the moderator performance simulation for the current instrument suite, in particular for the set of instruments viewing the coupled-cold moderator on SPTS. Because of the premature suspension of the ESS technical work, this next iteration cycle has not yet been performed, i.e. possible improvements through design changes based on the results presented in chapter 4 has not been looked into by the ITG.

5.2 PROGRESS, NOVELTIES AND IMPROVEMENTS

The expected neutronic performance of the ESS design allows for novel instrumentation. Two examples of new concepts are ultra-high resolution powder diffraction (URPD) and small angle scattering at very low momentum transfer (VSANS). With URPD a resolution comparable with that of synchrotron radiation is within reach, enabling much enhanced synergy of the two radiation probes in condensed matter research.

VSANS extends the Q-range in 2D small angle scattering to unprecedented small values. Advanced instrumentation at LPTS will take advantage of wavelength band-width multiplexing and frame replication techniques. Ballistic guides will be used to transport neutron beams with little losses over large distances and at relatively low cost. Without the huge intensity penalty for a long instrument more efficient designs, utilizing a larger fraction of the neutrons produced in the target can be made.

At ESS all beam lines should have very similar geometric design and individual wheel drum shutters (figures 4.5.2.1, 4.5.2.2, 4.5.3.6). No guide bundles or split beam lines are planned at present. The distance between the moderator surface and beam line front end has been minimized, the shutters can accommodate individually designed front-end neutron guides for the specific need of each instrument. The separation angle between adjacent beam lines is kept as small as technically feasible. The wheel drum shutter design of ESS (chapters 4.5.2, 4.5.3) allows for a 1.6m gap between moderator and front beam optics at 11° separation angle and a total of 22 individual ports covering approx. 240°. The wheel drum shutters offer a wide open cross section for variable and easy to access front-end beam optics.

Table 5.2.1: ESS front-end beam-line design parameters and tolerances

No. of viewing fans per target station, total coverage angle	4, >240 deg
No. of beam lines per fan	6 (the resulting total of 24 beamlines / target station is reduced to 22 + 2 horizontal moderator access lines.)
Beam line separation angle	11 deg, with individual wheel drum shutters
Min. distance between moderator surface and guide front end	~ 1,6 m
Length of front n-guide (shutter wheel diameter)	2,8 m
Outer cross section of inserts:	170 mm x 230 mm (height x width)
Inner net cross section of inserts:	150 mm x 190 mm (height x width)
Required active cooling of insert:	no
Max. temperature of surrounding structure:	150° C
Horizontal displacement tolerance	0.3 mm
Vertical displacement tolerance	0.3 mm
Horizontal angular alignment tolerance	0.1 °
Vertical angular alignment tolerance	0.2 °
Reproducibility of inner insert position after open – close – cycle:	Same as tolerances
Exchange of inner insert:	access from top (vertical)
Maximum frequency of inner insert exchange:	~ once per year (radiation damage)
Exchange of outer insert:	access from instrument hall (horizontal)
Maximum frequency of outer insert exchange:	~ once per 10 years (change of instrument)

The bi-spectral moderator concept is based on a novel beam extraction system as proposed by Mezei and Russina [Mezei, 2002a] (figure 5.2.1). The instrument ends up viewing the cold part of a side-by-side cold-thermal moderator for the long wavelength neutrons and the thermal part for short wavelength. The concept utilizes the fact that a Si wafer is almost transparent to thermal neutrons and cut-off angle of its supermirror coating is proportional to the neutron wavelength. An example of the expected spectrum is shown in figure 5.4.2.

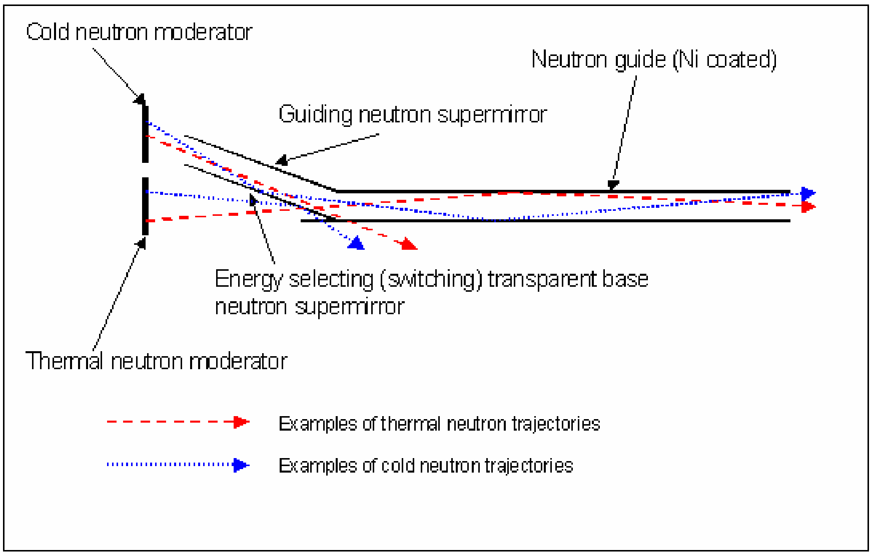

Figure 5.2.1: Novel proposal for a bi-spectral beam extraction using a deflected front-end cold guide on Si-wafer substrate. F. Mezei,M. Russina, (HMI), patent submitted in Berlin, 2002

For optimized intensity for a given resolution, a low-cost primary flight path with matched length is important for the design. Novel ballistic guides with a divergent / convergent front and back-end and a standard m=1 natural Ni coating at the center part allow for very efficient neutron beam transport over long distances at reasonable costs. In fact, for wavelengths λ>1Å the ballistic guide transmission exceeds that of a supermirror or standard Ni-coated guide substantially and is furthermore cheaper than integral supermirror coating. Figure 5.2.2 illustrates the design of a ballistic guide and figure 5.2.3 shows its transmission obtained from Monte-Carlo simulations.

Average number of reflections at 10Å:

SM guide	70
Ni guide	25
Ballistic guide	10

Figure 5.2.2: Design sketch of a ballistic neutron guide

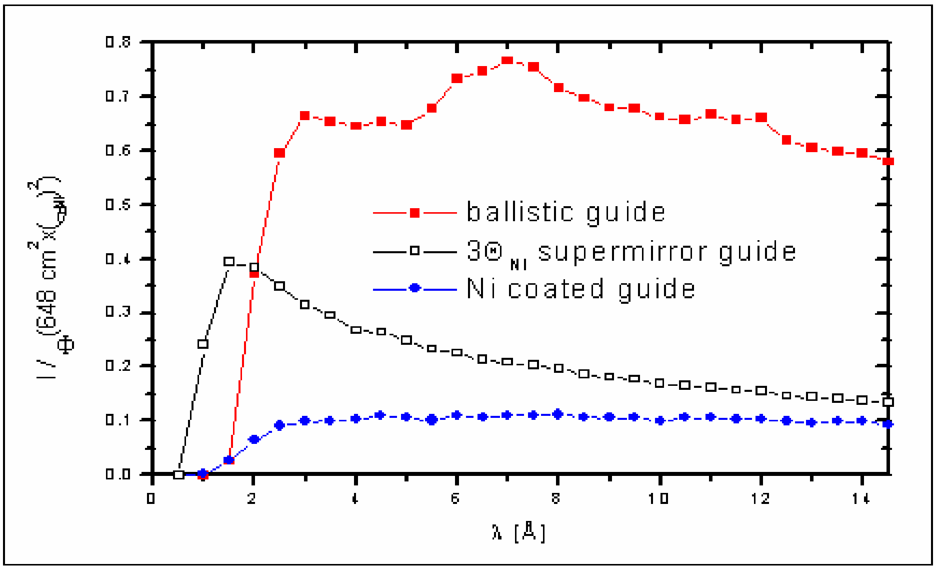

Figure 5.2.3: MC simulated transmission of a standard Ni coated, SM-3 and ballistic guide versus neutron wavelength

High-resolution powder diffraction is one of the main strong holds for the established pulsed spallation sources e.g. HRPD at ISIS. The high resolution is a consequence of the narrow pulse width of decoupled, poisoned cold moderators in the slowing down regime, i.e. for $\lambda < 1.8$ Å neutron wavelength (cf. tables. 4.1.3, 4.1.4). Mechanical choppers, however, can produce considerably shorter pulses for the major part of the wavelength range of interest: Fermi choppers can reach FWHM of < 5 µs and a counter-rotating pair of state of the art disc choppers < 10 µs. In the latter case the beam width at the chopper has to be about 1 cm, which is comparable to typical sample sizes in diffraction work. Modern neutron optical beam delivery systems allow us to refocus the beam to the sample or the chopper.

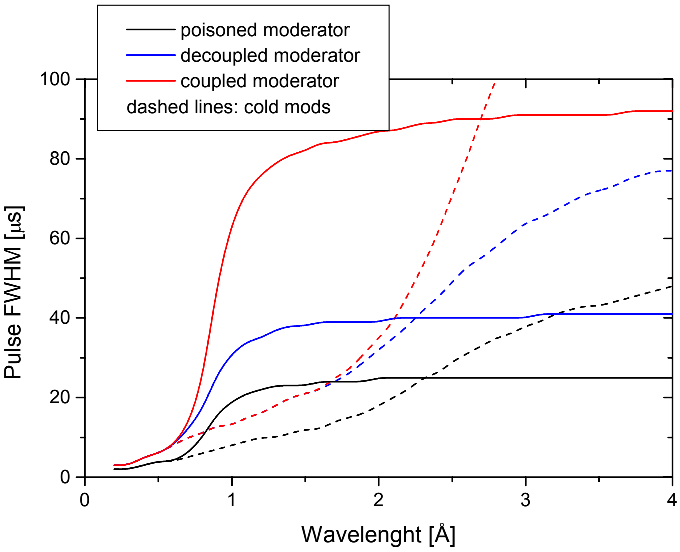

Figure 5.2.4: Typical FWHM pulse lengths for pulsed spallation source moderator options considerably exceeds for most wavelengths the 5-10 µs limit available by mechanical choppers. The precise values for a given moderator option on a specific source will depend on the engineering details cf. chapter 4.1

5.3 OPTIMIZATION OF THE SHORT PULSE TARGET STATION

The present engineering solution to the revised moderator design has now been studied by Monte Carlo simulations (chapter 4.1 and [Filges, 2003]) and the number of beam lines per target station was reduced from 24 to 22, to allow for horizontal moderator insertion (cf. table 5.3.1). The SP-instrument suite therefore needs to be readdressed and at minimum, a minor reshuffle will be called for. The prospects of future advanced moderators (cf. chapter 4.7, figure 4.7.1.4 and [Conrad, 2004]) in exchange for e.g. the side-by-side broad band-width conventional moderator might have a more profound influence on the instrument suite. Another aspect to be revisited is whether the set of instruments that request a high intensity coupled cold moderator on SPTS would do equally well with the bi-spectral moderator design. These aspects were not studied because of the premature stop to the technical work for the ESS project.

A detailed description of the fully simulated and high priority instruments is compiled in Vol. IV of the Bonn Conference documents [ESS, 2002a].

Table 5.3.1: Instruments at the Short Pulse Target Station (SPTS), High priority reference instruments are typed in red

Port no.	Instrument	Acronym	Moderator	Flight Path Length (m) (prim.L_i, sec. L_f)	Incident Energy (meV)	λ-range (Å)	SAC rating (Flagship/ Mission)
ST01	**Bottom Moderator Insert**						
ST02	**Thermal Chopper Spectrometer (medium resolution)**	**MET**	**TDC**	**14, 2.5**	**15-1500**	**0.23-2.5**	**9/8**
ST03	**Molecular Spectroscopy**	**TOSCA**	**TDC**	**17, 1.5**	**3-2000**	**0.2-5**	**4/7**
ST04	**High Resolution Single Crystal Diffractometer (chemical crystallogr.)**	**CHRSXD**	**TDC**	**15, 3**	**3-1300**	**0.25-5**	**2/3**
ST05	**High Q Powder Diffractometer**	**HQP**	**TDC**	**40, 2**	**1-10**	**3-8**	**5/10**
ST06	**Liquids and Amorphous Materials Diffractometer**	**LAD**	**TDC**	**11, 6**	**3-33000**	**0.05-5**	**5/1**
SM07	**Particle Physics Beam Line S**	**PPS**	**BS**	**40, x**	**–**	**–**	**–**
SM08	**–**	**–**	**–**	**–**	**–**	**–**	**–**
SM09	**High Resolution Protein Single Crystal Diffractometer**	**HRPSXD**	**BS**	**40, 2**	**3-25**	**1.8-5**	**3/0**
SM10	**Single Pulse Diffractometer**	**SPD**	**BS**	**10, 2**	**1-250**	**0.5-8**	**–**
SM11	**Medium Resolution Backscattering Spectrometer (5 μeV)**	**MRBS**	**BS**	**40, 2**	**1.6-20**	**2-7**	**–/4**
SM12	**High Energy Chopper Spectrometer (high resolution, low Q)**	**HET**	**BS**	**15, 8**	**15-1500**	**0.23-2.5**	**4/6**

Port no.	Instrument	Acronym	Moderator	Flight Path Length (m) (prim.L_i, sec. L_f)	Incident Energy (meV)	λ-range (Å)	SAC rating (Flagship/ Mission)
SD13	**Backscattering Spectrometer (17 μeV)**	**LRBS**	**CDC**	**30,2**	**1 – 80**	**1 - 9**	**–**
SD14	**eV Spectrometer**	**EVS**	**CDC (hot mod.)**	**12, 1**	**5000-64000**	**0.04-0.11**	**–/–**
SD15	**Tomography / Radiography Instr.**	**TOMO**	**CDC**	**25, 4**	**1.6-82**	**1-7**	**7/8**
SD16	**Engineering Diffractometer**	**ENGIN**	**CDC**	**50, 3**	**1.6-170**	**0.7-7**	**8/9**
SD17	**Magnetic Powder Diffractometer**	**MagP**	**CDC**	**50, 2**	**0.1-82**	**1.0-30**	**4/5**
SD18	**High Resolution Powder Diffractometer**	**HRPD**	**CDC**	**200, 2**	**0.3-170**	**0.7-15**	**13/14**
SC19	**High Resolution Backscattering Spectrometer (0.8 μeV)**	**HRBS**	**CC**	**200, 3**	**0.4-20**	**2-10**	**7/6**
SC20	**–**	**–**	**–**	**–**	**–**	**–**	**–**
SC21	**High λ Resolution SANS Instrument**	**HR-SANS**	**CC**	**12, 20**	**0.2-20**	**2-20**	**2/1**
SC22	**High Resolution Reflectometer**	**HRRf**	**CC**	**12, 3**	**1.6-20**	**2-7**	**8/11**
SC23	**Cold Chopper Spectrometer (low resolution)**	**LET**	**CC**	**40, 3**	**0.5-80**	**1-12**	**6/4**
SC24	**Top Moderator Insert**						

Moderator*: TDC thermal decoupled, BS bi-spectral, CDC cold decoupled, CC cold coupled

5.4 OPTIMIZATION POTENTIAL OF LONG PULSE TARGET STATIONS

The two-target station concept in ESS Project 2002 is making optimal use of the complementarity between the short and long pulses. Combining the two gives ESS a leading edge for all kind of neutron scattering experiments, both compared to existing and currently planned neutron sources [ESFRI, 2003]. In the original design (ESS-1996) the linac accelerator was optimized for short pulse operation and the long pulses were produced by the so defined linac without any essential change. This lead in particular to the 150 MW peak power of the linac (at 1.33 GeV final proton energy and 113 mA current) during 2 ms long pulses to achieve 300 kJ energy per pulse on the target. With the capability of shaping LPTS pulses into a variety of shorter and sharp pulses, as discussed below in connection with figure 5.4.4, this kind of use of the long pulses is the better served the higher the peak proton beam power and consequently the peak neutron flux is. Therefore, while for low wavelength resolution applications the energy per pulse is the relevant parameter for not too long pulses, other uses, such as URPD will benefit from compressing the same energy into shorter long pulses. To achieve this there is limited room to enhance the peak proton beam current, but the final proton energy in the linac can be further enhanced without essentially reducing the efficiency of neutron production per power delivered (cf. J-PARC project with 3 GeV final proton energy). Thus a linac optimized for LPTS use would rather aim for 2.5 – 3 GeV energy and 150 mA proton beam current. For long pulses alone there is no need to accelerate protons in the form of H^- ions, which is a more demanding task than producing and accelerating H^+ ions, i.e. bare protons (e.g. the vacuum requirements are less demanding). With these linac parameters 15 MW power in 16.67 Hz operation could be achieved, which implies nearly 3 times higher peak flux for the optimized LPTS than for the ESS 2002 reference design. Further work on the target should investigate whether significant increases in energy per pulse can be handled. Figures 5.4.1 and 5.4.2 show the gain in peak flux by going to higher linac peak power.

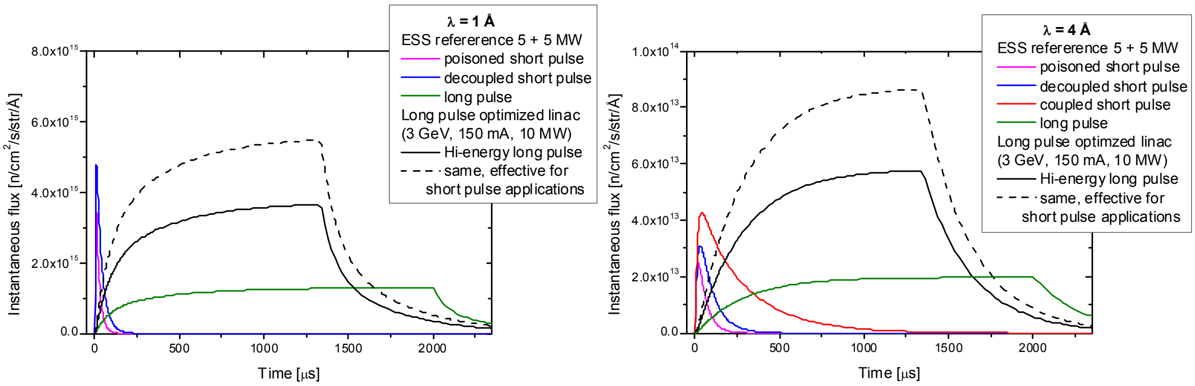

Figure 5.4.1: Neutron pulses from different moderators for the ESS 2002 5 MW SPTS + 5 MW LPTS reference design (colored lines) and for better optimized high energy long pulses (Hi-LPTS) with 1.333 ms pulse length for 600 kJ beam energy per pulse (black lines). The effective fluxes for short pulse applications (dashed lines) take into account, that at equal global instrumental resolution the sharper shaped LPTS lines (cf. fig. 5.4.4) will have larger FWHM than SPTS pulses with exponentially decaying tails.

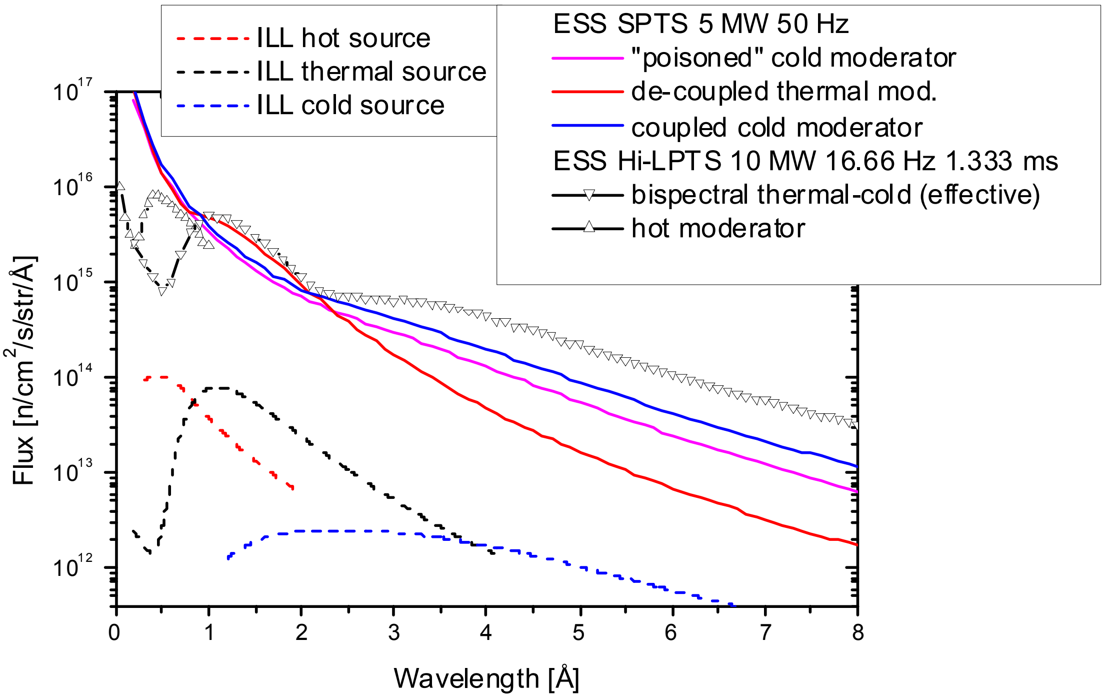

Figure 5.4.2: Peak fluxes of various ESS target station and moderator options, compared with the steady state flux of ILL moderators

5.4.1 High resolution and LPTS

The use of mechanical choppers was and is being envisaged in many cases for shortening moderator neutron pulses at short pulse spallation sources (existing or under construction) in time-of-flight inelastic spectroscopy, although it has not yet been practically tested. There is no principal technical difficulty to expect here, since with a single neutron velocity being selected from each source pulse, the opening of the pulse shaping chopper (necessarily outside the bulk shielding i.e. about 6 m from the source moderator) can be phased exactly to the time of passage of the neutrons with the desired velocity, at a given delay time after firing of the source. In diffraction type applications this unavoidable minimum distance between moderator and chopper has by now principally prevented mechanical pulse shaping. Indeed, even for a coupled moderator with 100 – 200 µs FWHM pulse length in the wavelength range 2.5 – 4 Å the pulse-shaping chopper at 6 m distance will reduce the transmitted wavelength band to 0.067 – 0.133 Å, which implies a proportional loss in data collection rate compared to the 0.8 Å band of an HPRD type instruments with 100 m moderator to detector distance at 50 Hz source frequency. Pulse shaping becomes a more feasible option for 1 – 2 ms duration long pulses (0.67 – 1.3 Å wavelength band), however, the lower repetition rate of the long pulse target station (LPTS) makes this still not sufficient. The principle of Wavelength Frame Multiplication with the help of multiplexing chopper systems has been invoked in [ESS, 2002b] as a solution to this problem. This approach has by now been worked out in detail [Mezei, 2002b].

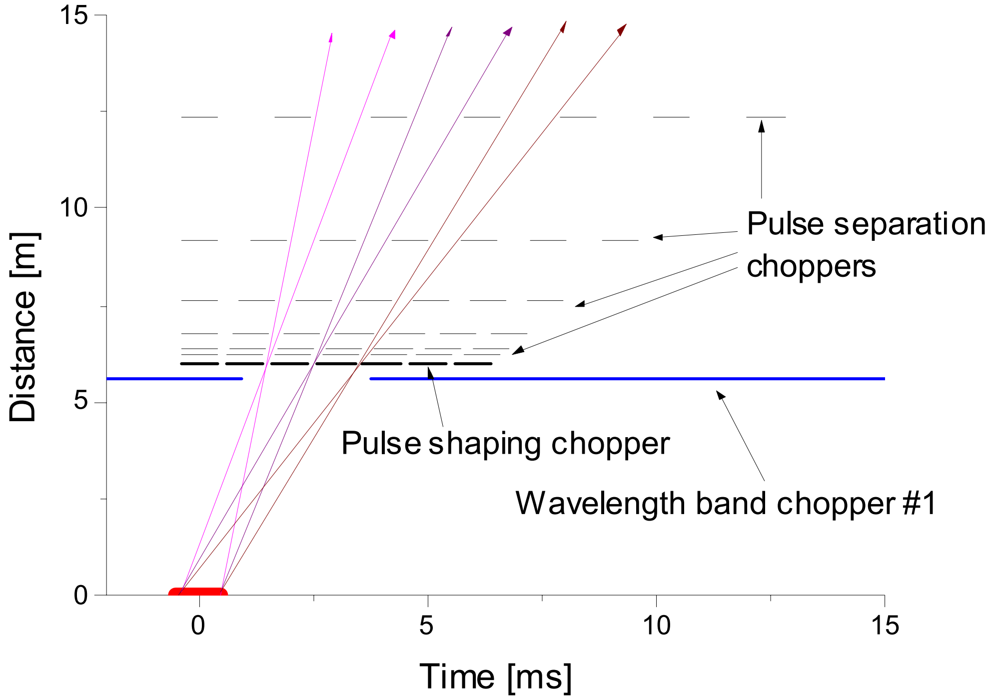

Figure 5.4.3: General pulse shaping method using multiplexing chopper system to overcome the reduction of the wavelength band by Wavelength Frame Multiplication method

As illustrated in figure 5.4.3, the wavelength frames defined by subsequent openings of the fast pulse shaping chopper (shown in different shades of purple) can provide a continuous coverage of the full wavelength band determined by the source frequency and the distance of the instrument (e.g. 2 Å band width in the example in the figure for 16.67 Hz and 120 m, respectively, with 1 ms useful source pulse length and 6 m moderator to pulse shaping chopper distance). The role of an ensemble of 4 – 7 pulse separation choppers downstream from the pulse shaping chopper is to make sure that the wavelength frames selected by different openings of the pulse shaping chopper do not overlap in time at the detector, with particular attention for neutrons coming from the long time tail of the source pulses with significant intensity from the point of view of background noise up to 5 – 8 ms. By slewing the common phasing of the pulse shaping and pulse separation choppers compared to the source timing one obtains on average the same smooth intensity distribution as a function of wavelength as in the conventional case without pulse shaping. The wavelength band chopper(s) (cf. figure 5.4.3) also operate in the usual, well-established fashion. In order to achieve full efficiency the pulse separation choppers must not interfere with the neutrons selected for use (i.e. they need to be disc choppers fully open when "good" neutrons are passing). Taking into account that it needs a finite time for these choppers to go from fully closed to fully open position, the scheme practically requires a minimum separation of about 0.8 ms between pulse shaping chopper pulses, which roughly equals the assumed source pulse length. Therefore, while this method offers a general tool for pulse shaping for all applications of long pulses, on a short pulse target station it would imply the restriction that the apparent source peak flux will be reduced to the average over a period of at least 0.8 ms from the beginning of the pulse. This eventually can be an acceptable loss in effective brightness for coupled moderator pulses in the fully thermalized wavelength regime with rms pulse lengths in the range of 0.2 – 0.5 ms.

This technique opens up the way for building high wavelength resolution instruments on the long pulse target station, in particular by making shorter pulses than those delivered by poisoned short pulse moderators available for neutron wavelengths > 0.9 Å (cf. table 4.1.4). For such wavelengths supermirror based ballistic guides can deliver neutrons with intensity gain compared to the direct view of the moderator. In view of the lower repetition rate of LPTS,

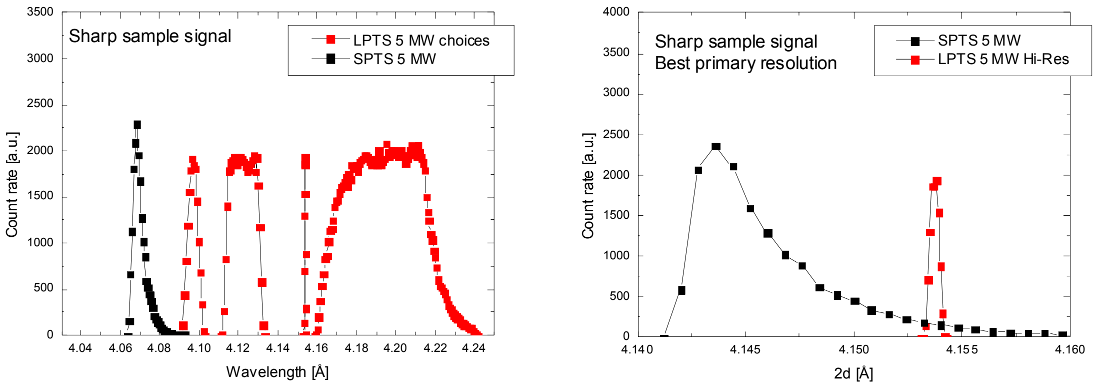

Figure 5.4.4: Powder diffraction options. Left hand side: Bragg line at the SPTS thin cold moderator (black symbols) compared with variable resolution lines obtained by different shaped pulse lengths on the LPTS cold coupled moderator. The right most signal is the LPTS signal without pulse shaping. Right hand side: comparison of the best incoming resolution options for both cases. The instrument lengths are 50 m and 150 m for SPTS and LPTS, respectively, and the shortest pulse shaping chopper pulse is 30 μs FWHM. (Computer simulation results)

longer instruments can be envisaged here while maintaining the wavelength band, which further enhances the incoming wavelength resolution. Substantial additional advantages of shaping of long pulses are the perfect line shape without slowly decaying exponential tail and the capability to adjust the resolution for the needs of each sample, in order to optimize the flux on the sample.

These potentials are illustrated in figure 5.4.4, by comparing the neutron diffraction line shapes for a perfect powder sample at high scattering angles to avoid additional resolution broadening. The simulated SPTS signal assumes poisoned (thin) cold moderator and 50 m source to detector distance. On the LPTS the coupled cold moderator is used with an instrument length of 150 m, i.e. in both cases the basic wavelength band of the instrument (without suppressing source pulses) is 1.6 Å. The flexibility of resolution and the sharper line shape make the data collection rate in the LPTS option in this wavelength range actually superior to the SPTS one, in spite of somewhat higher peak signal for the latter.

The right hand side of the figure illustrates the potential gain in resolution to realize Ultra High Resolution Powder Diffraction (URPD) in neutron scattering. This can be achieved on the LPTS by the combined effect of short chopper pulses and longer flight path at the same wavelength band. The ultimate limit for incoming wavelength resolution for lattice spacings $d > 1.5$ Å can attain $4*10^{-5}$, for sample sizes approaching the cm range, however, this can only be made full use of at scattering angles very close to the exact backscattering position (within about 1°). The example shown in figure 5.4.4 corresponds to $\delta d/d \sim 1.5*10^{-4}$, which can be more readily achieved.

5.4.2 Examples of new LP-instruments

5.4.2.1 Ultra-High Resolution Powder Diffraction (URPD)

The Ultra High Resolution Powder Diffraction (URPD) is aiming at $\delta d/d \sim 10^{-4}$, nearly an order of magnitude beyond current capabilities. This kind of resolution is common at synchrotron radiation facilities and experience has identified a number of prominent applications, for example the study of micro-strain, which can play an important role in phase transitions in real crystals. Being able to perform neutron and X-ray scattering experiments with comparable resolution in the future will open up new opportunities to make the most out of the synergetic use of both radiations. The technical realization is based on the pulse shaping technique for LPTS described in the previous chapter, 5.4.1.

5.4.2.2 Very Small Angle Scattering (VSANS)

In small angle neutron scattering (SANS) there is an emerging need to achieve minimal wave numbers in the10^{-4} Å^{-1} range, i.e. to improve resolution by an order of magnitude. In the most favorable technique, the conventional pinhole geometry, this would require improving the angular resolution from typically 0.05 – 0.1° to 0.005 – 0.01° (VSANS = very small angle neutron scattering), which implies for the same, already considerable instrument length a prohibiting 4 order of magnitude loss in neutron intensity. (For a Maxwellian neutron spectrum going to longer wavelengths leaves the intensity unchanged for a given Q resolution.) In the so-called Ultra SANS method, which has been implemented following Bonse and Hart and recently improved at several laboratories, in one dimension even smaller Q values have been achieved, but maintaining the 2 dimensional character of the pinhole techniques is seen as a crucial general requirement by the user community. For this reason 2D optical focusing techniques are being developed at several laboratories, which substantially reduce the abovementioned 4 order of magnitude intensity loss (by up to some 2 orders of magnitude), which will be further mitigated by the enhanced neutron beam power of ESS. Compared to steady state sources there is a major additional challenge for implementing VSANS: gravity makes neutron trajectories substantially wavelength dependent within reasonable pulsed source SANS wavelength bands (i.e. a few Å). E.g. 5 Å neutrons drop 2 mm over 10 m flight, and 10 Å ones twice as much. In comparison, the pinhole size at the sample needs to be 1 mm in order to achieve 0.01° resolution over 10 m collimation path. In addition, in the promising focusing techniques based on neutron refraction (hexapole magnets, solid state neutron lenses) the focal length is also wavelength dependent. Toroidal mirrors, in contrast, have fixed focus and the main consequence of gravity can be taken care of by moving up and down the beam stop in front of the detector, synchronously to the source pulses. To maintain best image quality, it is preferable to also move the incoming pinhole whose image is ideally projected on the beam stop, so that the mirror always is on the top of the parabolic neutron trajectories. In a somewhat similar fashion, converging collimators need to be synchronously "curved" to match the variation of the parabolic neutron trajectories. One way of achieving this is to make the neutrons "weightless" by oscillating the whole collimator synchronously to the source in the vertical direction imposing free fall acceleration over the time there are neutrons in the collimator (about 70 % of the pulse repetition time). The amplitude of the free fall motion only needs to be about 3 mm for a 16.6 Hz source. Figure 5.4.5 shows another alternative, namely to move elements of the collimator synchronously to the source in a fashion that for each wavelength a parabolic trajectory is selected which hits the sample and the beam stop in front of the detector at the same, constant height. It has also been suggested to use refractive prisms along the neutron trajectory to compensate gravity by bending the beam up-wards by an angle also proportional with the neutron wavelength. In sum, at a time when these focusing techniques for VSANS are vigorously being developed at several steady state neutron sources, approaches for their more challenging use on pulsed sources are also making progress.

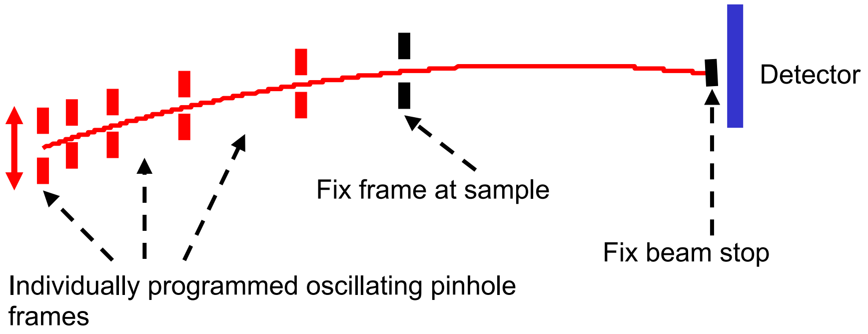

Figure 5.4.5: Compensating for neutron gravity effects for a converging collimator by vertically oscillating the pinhole frames forming the collimator. The maximal amplitude of motion is about 4 mm, well within the homogeneous area of an adequately shaped incoming beam

5.4.3 LPTS instrument table

A detailed description of the fully simulated and high priority instruments is compiled in Vol. IV of the Bonn Conference documents [ESS, 2002a]. A short summary is given in Table 5.4.3.1.

Table 5.4.3.1: Instruments at the Long Pulse Target Station (LPTS)
High priority reference instruments are in red

Port no.	Instrument	Acronym	Moderator	Flight Path Length (m) (prim.L_i, sec. L_f)	Incident Energy (meV)	λ-range (Å)	SAC rating (Flagship/ Mission)
LM01	Bottom Moderator Insert						
LM02	Variable Resolution Cold Neutron Chopper Spectrometer	VarChop	BS	90,3	0.2-80	1-20	5/2
LM04	High Intensity SANS Instrument	HiSANS	BS	21,30	0.2-20	2-20	15/22
LM05	Ultra-high Resolution Powder Diffractometer	URPD	BS	300,3	3.3-100	0.9-10	–
LM06	High Pressure Diffractometer	HiPD	BS	40,6	3.3-300	0.5-10	–
LC07	Neutron Depolarisation Instrument	n-DEPOL	CC	12,2	–	–	–
LC08	Grazing Incident SANS Instrument	GISANS HiRef	CC	20,8	0.2-80	1-20	–
LC09	Single Peak Diffractometer (CryoPAD)	SPAD	CC	20, 2	3-330	0.5-5	–/–
LC10	Very High Intensity SANS Instrument	SANS	CC	21,15	0.1-20	2-25	–
LC11	Fourier Diffractometer	FourDif	CC	25,2	0.2-80	1-20	–
LM13	Low Resolution Single Crystal Protein Diffractometer	LRPD	BS	20,2	0.3-3.3	5-15	2/4
LM15	Coherent Excitation Spectrometer (TAS)	TAS	BS	30,2	0.8-170	0.7-10	–
LM16	Wide Angle NSE Spectrometer / Diffuse Scattering Instrument	WanNSE	BS	50,4	0.1-20	2-25	2/2
LM17	High Magnetic Field Instrument	HiMag	BS	50,2	1- 80	1 - 9	–
LC19	Particle Physics Beam Line L	PPL	CC	40, x	0.1-20	2-25	–
LC21	High Intensity Reflectometer	HiRef	CC	37,3	1-20	2-9	8/3
LC22	Focusing Mirror Low Q SANS Instrument	FocSANS	CC	20,8	0.7-3.3	5-12	4/2
LC23	High Resolution NSE Spectrometer	HRNSE	CC	30,6	0.1-20	2-25	5
LC24	Top Moderator Insert						

Moderator*: BS bi-spectral, CC cold coupled
The five remaining neutron ports LM 03, LC 12, LM 14, LM 18, LC 20
are kept free for future instruments.

5.4.4 ESS generic instrumentation footprint

As a result of the science based definition and selection of the ESS instrument suite a major review and redesign of both, the moderator concept and target station geometry was undertaken (in comparison to the ESS 1996 proposal). Accompanying MC based neutronic performance calculations indicate that the proposed modifications are feasible and the performance expectations from the instruments likely to be satisfied. Thus, the new ESS target and moderator design provides numerous advantages that are described in detail, above. Figure 5.4.6 illustrates the proposed footprint of the ESS instrument suite.

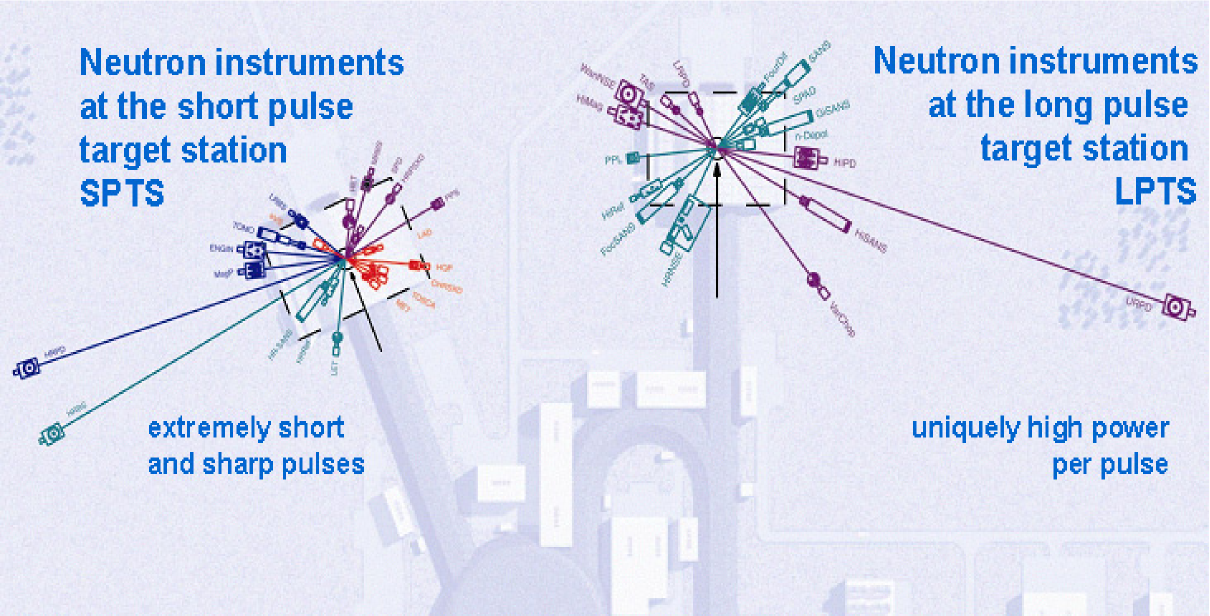

Figure 5.4.6: Footprint of the proposed ESS instrument suite as a result of the target-moderator and instrument interface iteration process

5.5 TOTAL FACILITY PERFORMANCE AND *ESFRI* EVALUATION RESULTS

A SAC and ESFRI working group [ESFRI, 2003] evaluated the total performance of the proposed ESS instrument suite of both target stations. This was done in comparison to other existing neutron research facilities, namely the ILL and ISIS, and in comparison to the future competing sources SNS and JPARC. Moreover, the relative importance of every individual instrument was evaluated and it expected impact for the eight research themes and scientific missions of ESS as SAC defined them [ESFRI, 2003]. ESS will in all cases be World-leading, in some cases even by a considerable margin.

5.6 GENERIC DEVELOPMENTS

The development of new instrument components and instrumentation techniques progresses rapidly fuelled by the desire to maximise the efficiency of neutron scattering instruments on existing sources. Indeed the ESS instrument designs have only become possible over the last few years, and further gains in instrument performance might be anticipated as these developments continue. The EU FP6 NMI3 programme helps to support important collaboration between European Neutron Centers.

Developments in guides and optics, choppers and data acquisition are essential if the full potentials of next generation sources such as the ESS are to be realized. Developments of detectors, polarization and software are particularly important.

5.6.1 Detectors

The high fluxes that will be available at the ESS will pose challenges that cannot be easily met using the detector technology that is available today. In addition, many of the instrument designs impose stringent requirements on detectors to provide high spatial resolution in two dimensions and high time resolution.

The likely requirements for ESS detectors are

- Very high-count rates of up to $2x10^5n.s^{-1}cm^{-2}$ must be handled.
- Large detector areas at reasonable cost.
- High spatial resolution and time-of-flight resolution.

Current detector programmes are being pursued at the European neutron centres and collaborative projects also exist with laboratories in the US and Japan, where the SNS and J-PARC respectively are requiring similar detector developments. For the ESS it is vitally important that this development work continues, with focus on new detector technologies required for the ESS. Detector development will continue under the NMI3, EU FP6.

Developments in the following areas will be of particular importance.

- Micro-strip gas detectors – a range of systems are being developed.
- Hybrid micro-pattern detectors
- Scintillator materials with improved efficiency and γ sensitivity.
- Highly-pixelated transmission detectors for tomography.

5.6.2 Polarisation

Polarisation analysis is likely to be a required option for many of the instruments on the ESS, rather than only on a selected few, providing the technology has progressed sufficiently. Good progress is being made in the development of ^{3}He filter technology and in the use of supermirror polarisers. In particular the new opportunities of achieving higher level of ^{3}He polarisation than thought possible until recently will provide major improvements in the efficiency of neutron polarisation.

Two programmes are being pursued under MNI3; the Polarized Neutron Techniques network led by FZ Jülich and the Neutron Spin Filters network led by the ILL. The networks comprise Europe‘s leading experts in the field with good links to groups in Japan and the US. The networks showed ensure that the current momentum in the development of neutron polarization is maintained.

At the PNCMI workshop in Jülich in September 2002 working groups were convened to discuss the opportunities for polarised neutron scattering on next generation neutron source. Papers arising from these discussions have been published in the proceedings of that conference.

5.6.3 Software

The current trend at existing neutron source is a steady increase in data volumes fuelled by the increasing use of highly pixilated detectors and parametric measurements. With the flux increases available on next generation sources data volume and rates will increase dramatically, placing increasing demands on the analysis software. A broadening User Community, with an increasing proportion of 'non-expert' users will require greater automation from the analysis software and capability for remote access.

Development programmes are being established in the US and Europe to ensure that software developments are able to match the requirements. Distributed computing systems are likely to become increasingly important along with the development of more sophisticated data visualization tools.

Monte Carlo instrument simulation has played a vital part in the development of the ESS reference instrument suite. It is important that development work continues in this area under the aegis of NMI3. The use of simulation in experiment planning and control will be important to high flux pulsed sources.

5.6.4 TOF instrument developments at EU neutron centers

Different beam focusing methods are being developed and tested at various European laboratories, with the primary motivation to establish the VSANS approach for routine use at a number of steady state sources in order to improve the resolution in 2 dimensional (pinhole) SANS experiments compared to the current state-of-the-art limit of about 10^{-3} Å^{-1}. FZJ has achieved very encouraging results with a focusing toroidal mirror system, LLB and HMI is in the process of developing VSANS instruments using focusing systems based on converging pinhole collimators (variants of converging collimators have been developed earlier by several laboratories, including ILL) and BNC is working on hexapole magnetic lenses. These developments will establish crucial know how for implementing VSANS on ESS.

HMI and BNC collaborate since 1996 on the development of chopper systems for high-resolution time-of-flight powder diffraction both at steady state and long pulse spallation sources. A prototype has been built and tested with full success in 1999 at the Budapest research reactor and it is being currently converted to an instrument for routine user operation. The Extreme Environment Diffractometer (EXED) currently being built at HMI is an advanced version of the prototype with ultra-high resolution capability of $\delta d/d \sim 2.4*10^{-4}$ for $d > 1.5$ Å. This instrument, although optimized for use on a steady state reactor, will provide direct experience in this new resolution domain of neutron diffraction both in terms of science case, synergy with synchrotron X-ray work and the use of complex chopper systems and advanced neutron optics on long pulse spallation sources, optimization of data collection strategies and data analysis. More generally, quite some experience in advanced instrument concepts and techniques for ESS can be derived as much from developments at steady state sources as at pulsed sources.

At ISIS the focus of instrument development is directed on instrumentation for the Second Target Station (TS-2) which is currently under construction. It is envisaged that the initial instrument suite will comprise a multi-chopper spectrometer, three reflectometers, a SANS instrument, a disordered materials diffractometer and a powder diffractometer optimized for magnetic structure determination. Five of these instruments will view coupled moderators, consequently their design provides valuable experience in an important area for the design of ESS instruments. Development of high-speed disc choppers will be required for the multi-chopper spectrometer and ongoing detector development will be critical to most TS-2 instruments at ISIS.

The construction of the MERLIN chopper spectrometer at ISIS is now underway. The design has deviated from the norm in that the resistive wire ^{3}He are located inside the vacuum tank, thereby eliminating gaps in the detector coverage caused by structural struts and eliminating scattering from vacuum windows. The detectors are 3m long which also eliminated horizontal gaps in the detector array. The success (or failure) of these developments will inform instrument designs for the ESS.

5.6.5 Participation in projects overseas

Two MW spallation sources, SNS and J-PARC are in advanced stages of construction outside Europe. Collaboration with these emerging facilities will provide invaluable practical experience in a number of crucial areas, in particular in engineering and material issues in target design. The first, basic set of instruments on these sources is largely based on existing experience at ISIS and other current spallation sources, but there is a growing interest in more innovative approaches, which will open up new opportunities for advancing our know how. There are advanced plans for building a beyond state-of-the-art Neutron Spin Echo instrument at SNS under the leadership FZJ. Other innovative extensions of the SNS instrument suite based on ESS developments are also to be explored.

5.7 CONCLUSION AND OUTLOOK

In conclusion, progress in instrumentation concepts and components and higher linac power, primarily achieved by raising the proton energy to 3 GeV (similarly to the Japanese plan) allows us to further enhance the performance of ESS compared to the 2002 reference design. High power H^+ linacs up to 15 MW, see chapter 1.6 will make possible to enhance the performance of the long pulse target station, while the ESS 2002 reference design was already aimed at the probable limits for SPTS. The optimized LPTS offers both higher neutron flux per pulse for the low wavelength resolution typically “long pulse” applications (including single crystal studies with hot neutrons) and enhanced peak flux compared to SPTS for medium or high wavelength resolution typically “short pulse” applications for wavelengths $\lambda > 0.9$ Å. The optimized LPTS and the SPTS remain complementary, however with modified domains of best performance for each compared to the ESS 2002. Figure 5.7.1 compares data collections rates for 10 priority applications defined by the ESS SAC on the basis of input from the neutron scattering community for a variety of existing and planned neutron sources. It shows that ESS will represent a new leap in performance, especially for cold neutron and soft matter research compared to what is elsewhere envisaged today.

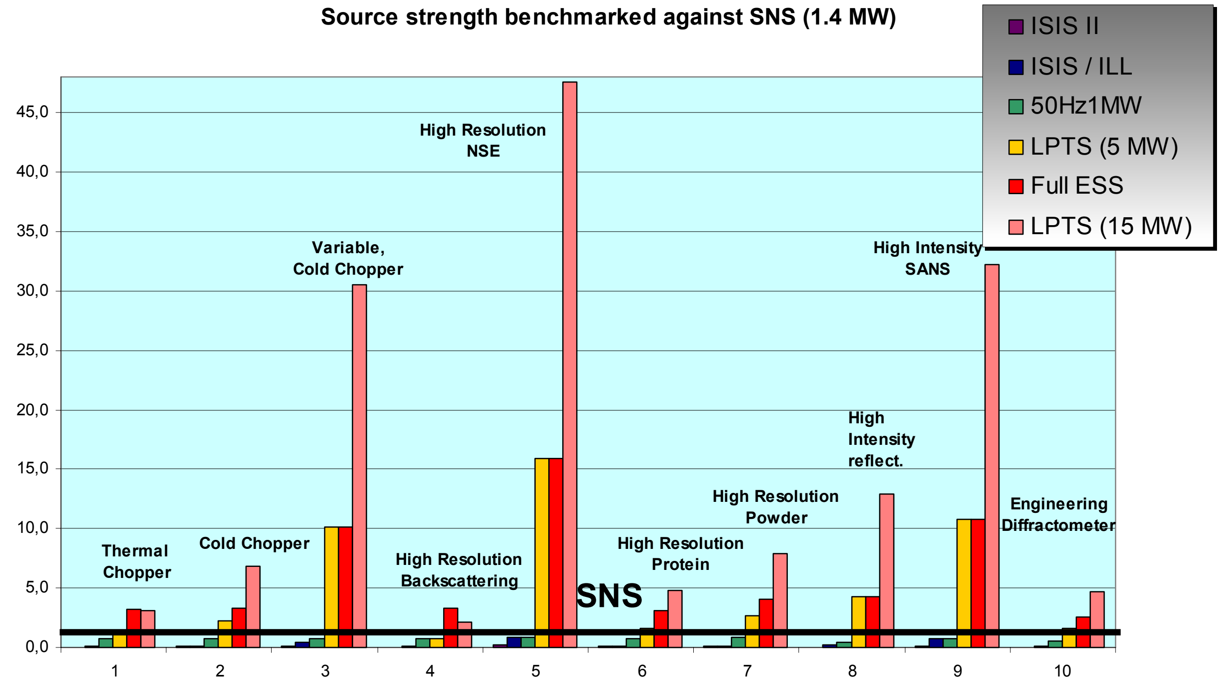

Figure 5.7.1: Comparison of the source performance for a number neutron source options, existing, under construction or planned in a set of 10 priority applications selected by the ESS SAC. The consequence (and thus feasibility) of raising the power to 15 MW on a LPTS target station has not been examined yet.

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