MEMORANDUM

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Subject: Vanadium standards for sample flux calibration on HYSPEC

This short note outlines design considerations for the Vanadium standard samples for neutron flux calibration on HYSPEC.

The standard way of calibrating the incident neutron flux at the sample position consists in measuring the scattering from the standard sample whose scattering properties are well understood and documented. The following important requirements need to be satisfied

1. the sample has to have known amount of scattering centers with known cross-section
2. the sample has to have well-defined geometry, covering the region of interest in the beam
3. the sample needs to be homogeneously illuminated in the beam, so that neutron flux is approximately the same for all scattering centers in the sample; if needed, the appropriate account for the beam penetration geometry should be performed

The standard scattering material most commonly used in neutron scattering is Vanadium. In order to properly design Vanadium standard one has to consider neutron beam extinction as it penetrates the V material.

For the range of energies of interest for the HYSPEC operation, the neutron beam extinction length in a flat Vanadium plate is in the range from ~ 0.8 cm to ~ 1.8 cm (Appendix). Using the geometric mean estimate for the average sample illumination by the inhomogeneous beam, we can estimate that for the illuminating intensity to be on the average roughly αI_0, where I_0 is the incident beam intensity, the transmission of the sample must be $\approx \sqrt{\alpha}$. Hence, for α of 95% (90%), a transmission of ≈90% (≈80%) is needed. The corresponding thicknesses of V are listed in the Table 2 of Appendix.

We finally estimate that in order to achieve an average 90% illumination of the V standard sample by the HYSPEC neutron beam we thus need an annular cylindrical sample with the wall thickness of 1 mm. For the 95% illumination the wall thickness of ≤ 0.5 mm is needed.

Vanadium standard samples of 0.5" and 1" outer diameter and with the height such that a section of 0.25" to 2" height could be exposed to the neutron beam, centered at its axis. These could be either man8ufactured by drilling out the inner part of V rod, or, by rolling an appropriate cylindrical shape of a piece of < 0.25mm thick V foil. In either case the samples have to be weighted so as to document the total # of V atoms, and mounted in a way which allows a well-defined predetermined amount of V to be exposed.

Appendix. Neutron beam extinction in Vanadium plate sample.

For the purpose of estimates we consider a plane-parallel V plate illuminated by the neutron beam normal to its surface. In order to determine the percent of the initial beam transmitted as a function of the thickness of the vanadium target, we first must note that the intensity of the incident beam will decay exponentially as a function of the thickness and the effective cross section [1]:

$$I = I_0 e^{-\mu_V t} = I_0 e^{-t/l_V}, \tag{1}$$

where I_0 is the initial intensity of the beam, and $\mu_V = 1/l_V$ is the effective cross section per unit volume for vanadium (l_V is the beam extinction length in bulk Vanadium),

$$\mu_V = \left(\sigma_{V,coh} + \sigma_{V,incoh} + \sigma_{V,abs}(E)\right) \cdot n_V. \tag{2}$$

Here n_V is the density of Vanadium atoms in the sample. For estimates we can use the crystallographic density, $n_V = N_V/V_V$, where $N_V = 2$ is the number of atoms per unit cell (2 atoms per body centered cubic unit cell of crystalline Vanadium), and $V_V = 27.818 \, \text{Å}^3$ is the volume of one unit cell of crystalline vanadium. This gives the atomic number density $n_V = 7.2 \cdot 10^{22} cm^{-3}$, corresponding to the weight density $\rho_V = 6.08 g/cm^3$. This compares well with the actual physical density of Vanadium of $6 \, g/cm^3$.

$\sigma_{V,coh} = 0.0183$ barn and $\sigma_{V,incoh} = 5.08$ barn are the coherent and incoherent cross sections of vanadium respectively [2]. $\sigma_{V,abs}(E)$ is the absorption cross section of vanadium, which is dependent on the energy of the incident beam. For most elements, the absorption cross section is proportional to 1/v (v = neutron velocity). The absorption cross section can be given obtained from that for the "standard" v = 2200 m/s thermal neutrons [b] (T = 293.58K "room temperature" neutrons with energy E ≈ 25.3 meV) using

$$\sigma_{V,abs}(E) = \sigma_{V,abs}(25.3 \, meV)\sqrt{\frac{25.3}{E(meV)}} = 5.08\sqrt{\frac{25.3}{E(meV)}} \quad \text{barn}. \tag{3}$$

In order to avoid the need to correct for the inhomogeneous sample illumination (beam extinction in the sample resulting from scattering and absorption), we have to limit sample thickness intercepted by the neutron beam to be significantly less than the extinction length l_V. Table 1 shows V absorption cross-sections and extinction lengths for several incident neutron energies in the HYSPEC typical range.

Table 1. V absorption cross-section and extinction length for several neutron energies.

E (meV)	5	10	15	20	30	40	60	80	100	120
$\sigma_{V,abs}$(bn)	11.427	8.080	6.597	5.713	4.665	4.040	3.298	2.856	2.555	2.332
μ_V (cm^{-1})	1.188	0.9474	0.8408	0.7773	0.7019	0.6570	0.6037	0.5719	0.5502	0.5342
l_V (cm)	0.8416	1.0554	1.1892	1.2864	1.4246	1.5220	1.6564	1.7484	1.8173	1.8718

It is clear from the last row that beam suffers roughly a factor 3 attenuation passing through V thickness of about 1 to 2 cm. Hence, V standard sample has to be significantly thinner than this in order to be fully illuminated. To determine the thickness as a function of transmission percentage we solve Eq. [1] for THICKNESS,

$$t = l_V log\ (I_0/I).\qquad\qquad(4)$$

Table 2 shows results for the potential thicknesses of the vanadium target for a selection of initial beam energies E and transmission percentages I/I_0.

Table 2. V thickness (mm) for a given transmission for several neutron energies.

E (meV)	5	10	15	20	30	40	60	80	100	120
$I/I_0 = 0.99$	0.085	0.106	0.120	0.129	0.143	0.153	0.166	0.176	0.183	0.188
$I/I_0 = 0.95$	0.432	0.541	0.610	0.660	0.731	0.781	0.850	0.897	0.932	0.960
$I/I_0 = 0.9$	0.887	1.112	1.253	1.355	1.501	1.608	1.745	1.842	1.915	1.972
$I/I_0 = 0.85$	1.368	1.715	1.933	2.091	2.315	2.474	2.692	2.842	2.954	3.042
$I/I_0 = 0.8$	1.878	2.355	2.653	2.871	3.179	3.396	3.696	3.902	4.055	4.177

References:

[1] Willis, B. T. M. and Carlile, C. J., 'Experimental Neutron Scattering', Oxford University Press, Oxford (2009).

[2] Sears, V. F. (1992) Neutron News 3, 26-37. "Neutron scattering lengths and cross-sections."