DESY Summer Student Programe 2008 Hamburg

Work report

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1 Introduction

My main work during the Student Summer Program 2008 at Hasylab in DESY was to prepare theory and create a new program to calculate x-ray absorption for liquid samples.

2 Theory

The detection system for a transmission EXAFS experiment is given in Fig 1a. The ionization chamber have absorption coefficients μ_1 and μ_2, with chamber lengths x_1 and x_2 respectively. The sample has a thickness x_s and a linear absorption coefficient μ_s. I is the total number of photons collected per data point entering the first ionization in the chambers, while I_1 and I_2 represent the signals arising from the ionizations in the chambers.

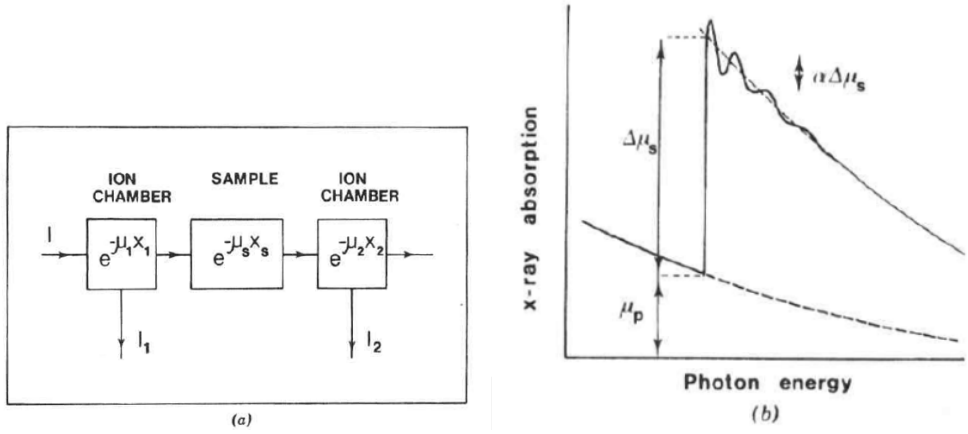

Figure 1: a) Detector system for EXAFS in transmision mode. b) An x-ray absorption spectrum.

The absorption coefficient of the sample can be calculated from $I_2/I_1 = exp[-(\mu_a x_s)']$. Due to the absorption coefficients of the ionization chambers, which enter in the measured signal I_1 and I_2, the determined absorption coefficient $(\mu_a x_s)'$ is not exactly equal to $\mu_a x_s$. The noise N in $(\mu_s x_s)'$ is given by:

$$N = \sigma(\mu_a x_s)' = [(I_1)^{-1} + (I_2)^{-1}]^{1/2}$$

Assuming that the amplitude of the EXAFS signal is equal to a fraction α (the normal range for α os $0.01 < \alpha < 0.1$) of the edge jump $\Delta\mu_s x_s$ (Fig. 1b) the normal signal S can by represented by $S = \alpha\Delta\mu_s x_s$. The relation between the signal-to-noise ratio (S/N) and I can be derivered:

$$\frac{S}{N} = \frac{I^{0.5}\alpha\Delta\mu_a x_s}{\{(1 - exp[-\mu_1 x_1])^{-1} + exp[\mu_a x_s + \mu_1 x_1](1 - exp[-\mu_2 x_2])^{-1}\}^{0.5}}$$

An optimum S/N is obtained with $\mu_1 x_1 = 0.25$, $\mu_2 x_2 = \infty$ and $\mu_s x_s = 2.55$.Using these values, we obtain the total number of photons I necessary to get a ceration signal-to-noise ratio (S/N) after t seconds collection time per data point:

$$I = 3.2(S/N)(\frac{\mu_s}{\alpha\Delta\mu_s})^2$$

The primary interacion of low-energy x-rays with in mattery, viz photoabsorption and coherent scattering, have been described for photon energies outside the absorption threshould regions by using atomic scattering fractors, $f = f_1 + f_2$. The atomic photoabsorption cross section μ_a may by readily obtained from the values of f_2 using the rlation:

$$\mu_a = 2r_0\lambda f_2$$

wher r_0 is the classical electron radius, and λ is the wavelenght. The index of refraction for a material with N atoms per unit volume is calculated by:

$$n = 1 - (f_1 + f_2)\frac{Nr_0\lambda^2}{2\Pi}$$

These (semi-empirical) atomic scattering factors are based upon photoabsorption measurements of elements in their elemental state. The basic assumption is that condensed matter may be modeled as a collection of non-interacting atoms. This assumption is in general a good one for energies sufficiently far from absorption thresholds.

In transmission EXAFS measurments sample inhomogeneities souch as pincholes and variation in thicknes be avoided. Although statistical consideration suport an optimum signal thickness of $\mu_a x = 2.6$, where $\mu_a x$ is the total linear x-ray absorption coefficient, thickness effectds arre less serious if $\mu_a x < 1.5$. For powdered samples with hight concentraction of the x-ray absorbing atom, the particle diameter D should by such that $\mu_a x \approx 0.1$ The cross-sectional area of the x-ray beam should by such less than thad of the sample and should by defined by appropriate mask preceding the I_0 chamber.

3 About program

Creating the new sample holder to liquid samples for x-ray measurements forced into writing the new control software. The program has an opportunity to appoint individual useful parameters to controlling new device (Fig. 2).

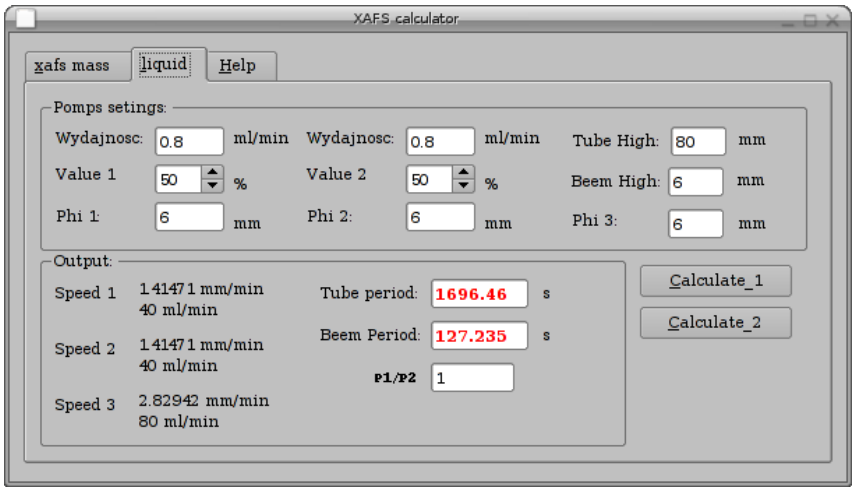

Figure 2: The main window, parameters of pomps and sample holder.

The program also has the function of appointing useeful of sample mass (Fig.3). A typical application is the calculate of the mass for a powder sample. The optimal sample thickness $\mu_a x = ln(I_1/I_0)$ depends on the absorption levels selected for the ionization chambers. Typically value $ln(I_1/I_0)$ is between 0.69 ($\mu_a x = 2$) and 1.09 ($\mu_a x = 3$).

Chemical formulas of compound should by entered in standard chemical notation (only chemical symbol), with appropriate and lower case. For example: the formula for copper sulfate must be entered $CuSO4$, parenrheses, spaces and dots may not by used. For example, the formula calcium phosphate must by entered as $Ca3P2O8$ (and not as $Ca3(PO4)2$).

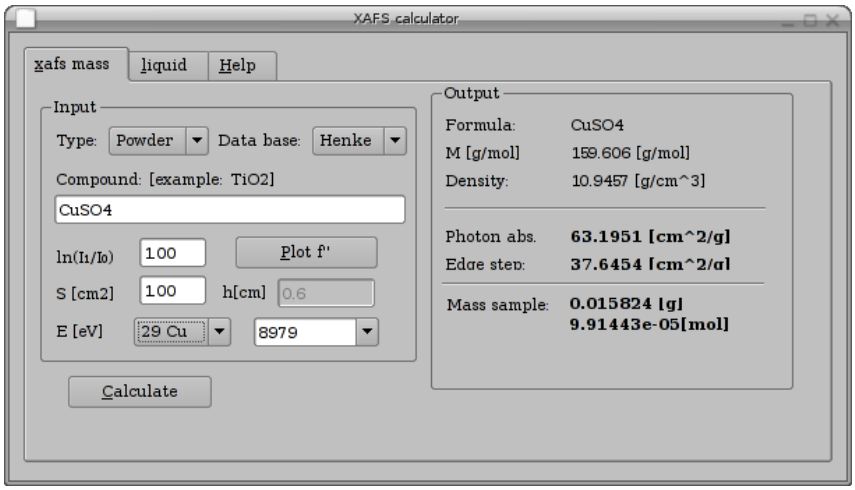

Figure 3: The main window.

4 Other activity

Another work during SSP, was testing a new sample holder to research chemical of liquid samples. Figure 4 presents the tested layout.

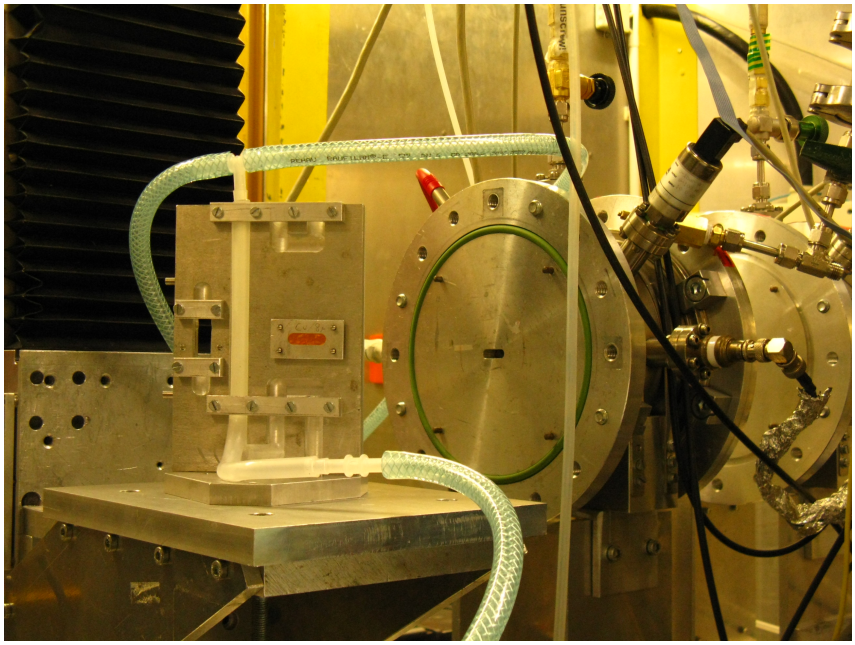

Figure 4: Sample holder instaled on beemline X1

My colleague and I from the group characterise the speed of pomps, differents between pomps and real speed of pumping for various parameters.

In the free time wy made pictures in hasylab and creat virtual 360^o panorams. Our work met with the approval, and in the future this panorams will by use to creat vitual tour around *Hasylab* and *PetraIII*