

Energy calibration using absorption spectral benchmarks

The calibration in energy of spectra can be done measuring well known and calibrated spectral features present in the absorption spectrum of the monitor mirror. This document shows how to calibrate spectra in energy using experimental data and the function matlab 'calibra.m'. As example, this document shows the calibration of spectra in the energy range between 50 and 100 eV. The calibration can be done by measuring the mirror current with the Si 0.1 μm filter of the beamline and using as spectral features the cutoff tails of the Si L edge at 1st and 2nd order (see Fig. 1).

In general, the user has to acquire 2 well known features (as the Si filter 1st and 2nd order tails) at the same deviation angle of measurements. The features have to be taken at two energies: the 1st one should be lower than the minimum of experimental data while the 2nd should be higher than the maximum. In case of a wide spectral range, it is better to take 3 spectral features.

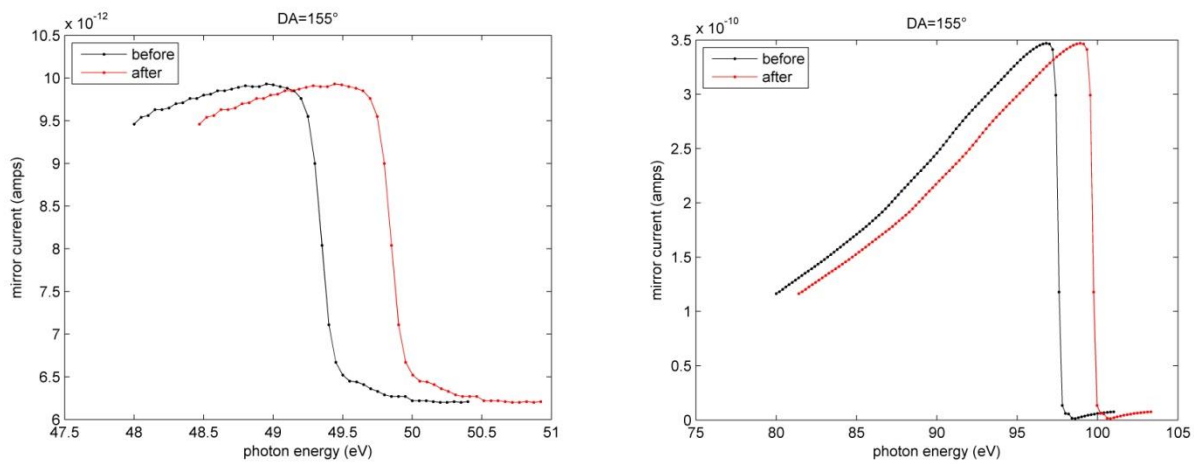


Fig. 1: Monitor mirror current around 50 eV (2nd order) and 100 eV (1st order) using Si filter. The black curves show uncalibrated spectra; red curves show calibrated spectra using the procedure here described.

The black curves of Fig. 1 show the absorption spectra with a well defined cutoff at about 50 and 100 eV, respectively 2nd and 1st order. The calibration of spectra can be done using the matlab routine 'calibra.m'. The function 'calibra' transforms energy data using a polynomial law. In case of calibration with two spectral features the polynomial degree is 1, in case of 3 spectral features the polynomial degree is 2.

The input parameters of the function calibra are respectively E_exp (experimental energy position of spectral features), E_real (real energy position of spectral features), n_pol (polynomial degree), E_old (experimental energy vector). The function 'calibra' output is the energy vector E_new (real energy output). (see red curves of Fig. 1). The code of the main matlab program and of the function 'calibra.m' are given below. The function – a) transforms all energies into wavelength values; b) it determines the coefficient of the polynomial relating experimental and real wavelengths using values given by E_exp and E_real; c) transforms output wavelength into energies.

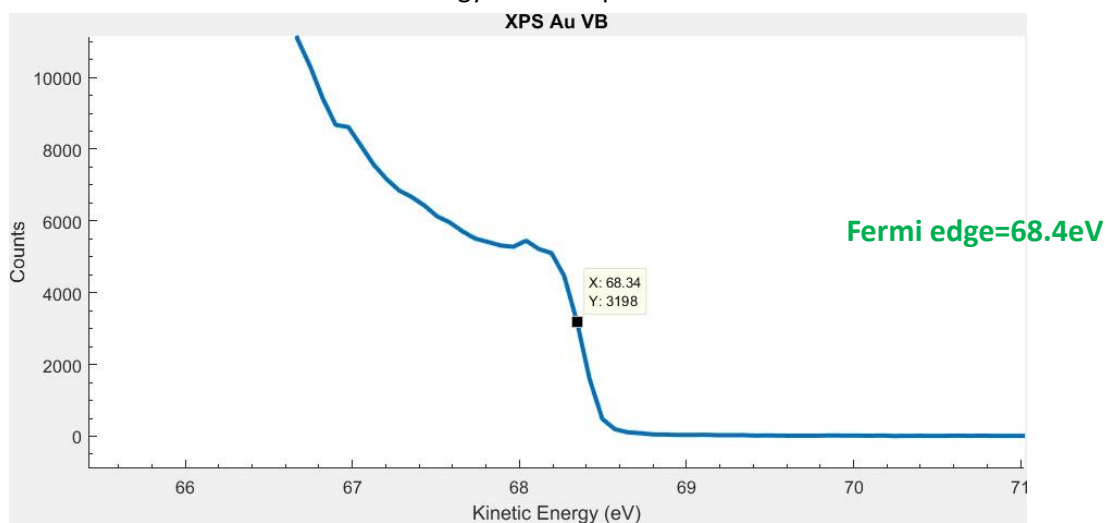
Features to calibrate spectra. All the features are present in the mirror monitor current. Most of the features have been taken inserting appropriate filters/windows. All the features have been calibrated using as a reference the Fermi edge of a Au 111 sample, except Al K edge.

Procedure of calibration

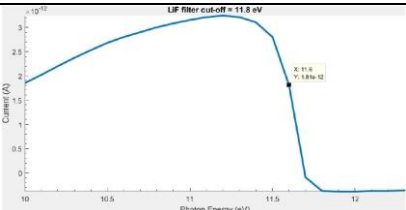
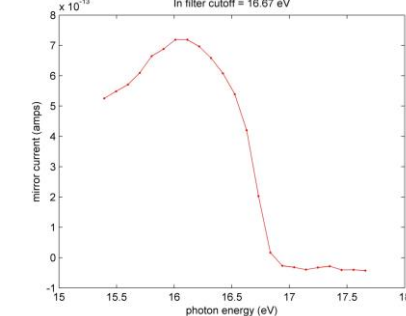
Energy calibration was performed by measuring Fermi edge of Au(111) crystal with electron analyzer, setting monochromator energy on various spectral features of REFO or filters cut-off

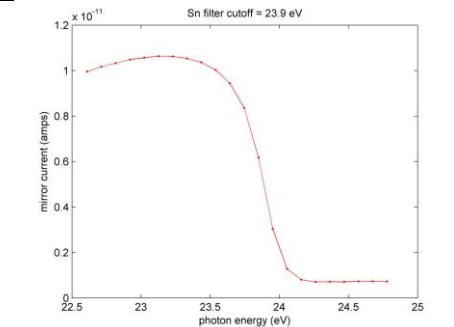
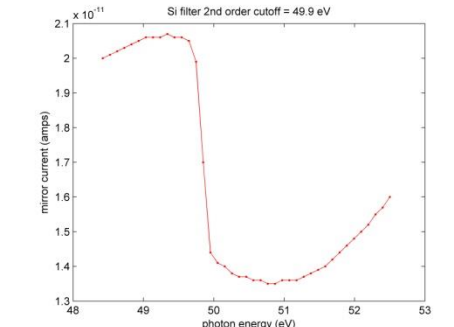
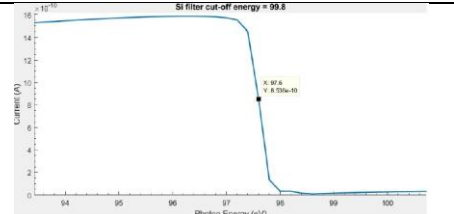
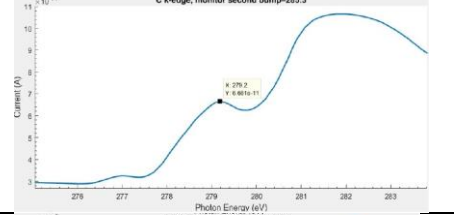
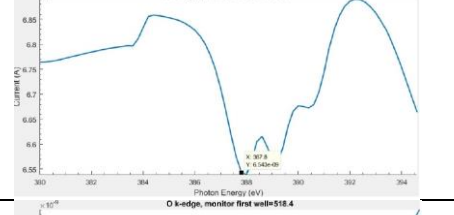
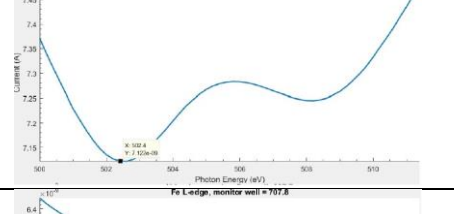
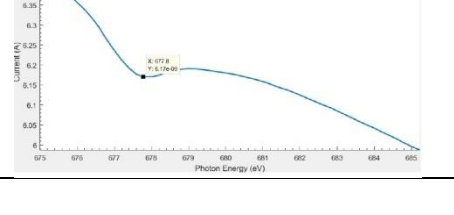
Example

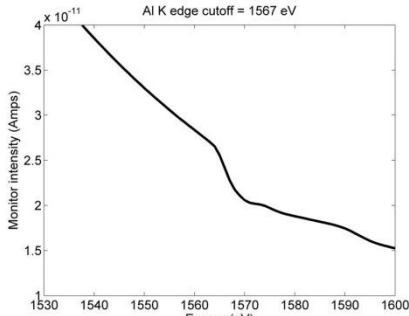
- From the next slide Al filter cut-off was defined as 71.5
- **Work function** of electron analyzer is known and checked: **4.3 eV**
- Monochromator set on 71.5 energy and XPS spectra of VB collected



- Real photon energy **68.4+4.3=72.7 eV**

Channel	Spectrum	Feature	Filter/window	Energy (eV)
GNIM		Li K edge	LiF	11.8
GNIM		In N edge	In	16.67

GNIM		Sn N edge	Sn	23.9
G1200		Si L edge (2 nd order)	Si	49.9
G1200		Si L edge (1 st order)	Si	99.8
G1200		C K edge	Full Beam	285.3
G1200		N K edge	Full beam	397.7
G1200		O K edge	Full beam	518.4
G1200		Fe L edge	Full beam	707.8

G1200		Al K edge	Al	1567
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Energy calibration verification G1200 (data september 2017)

Absorption edge, filter cut-off	Inclusion angle	Experimental value 1 (eV)	Experimental value 2 (eV)	Experimental value 3 (eV)	Calibrated energy value(eV)
Al cut-off	155°	71.5		71.7	72.7
Si cut-off 2 nd order	155°		49.4		49.4
Si cut-off	155°	97.6		97.9	99.8
	162°		98.3		
C edge	155°		275.2		285.3
	162°		277	277	
	164°		276.7		
	169,6°	279.2		280.2	
N edge	164°		381		397.7
	167°		386.5		
	169°		388		
	169,6°		387.8		
	172°	387.9			

Energy calibration verification G1200 (data september 2017)

Absorption edge, filter cut-off	Inclusion angle	Experimental value 1 (eV)	Experimental value 2 (eV)	Calibrated energy value(eV)
O edge	167°		500	518.4
	169°		501.2	
	169,6°		501	
	172.5°	502.4		
	173°		505.5	
Fe edge	172.5°	677.8		707.8
	173°		683.5	
	174.8°		685.5	
	175.8°		680.5	
Al edge	174.8°		1448	1560(?)
	175.8°		1418	

%% calling function %%%

E_exp=[97.55 49.35]; %experimental energy position of spectral features (in this case the half maximum of
%the Si absorption);

E_real=[99.7 49.85]; %real energy position of spectral features (in this case the half maximum of the Si %absorption.
This features have been calibrated by using Kr gas M absorption lines;

%n_pol=1; polynomial degree;

E_old; %experimental energy vector (x axis of Fig. 1);

E_new=calibra(E_old,E_real,E_exp,n_pol); % real energy output

%% calibra.m%%

function[Enew,coeff]=calibra(E,E_real,E_exp,n_pol)

L=1240./E; % transforms energies into wavelengths

coeff=zeros(n_pol,1);

if n_pol==1 % polynomial degree =1: to be used with 2 spectral features

if length(E_exp)==2

Mat=[1240./E_exp(1) 1

1240./E_exp(2) 1]; % matrix Mat

Vec=[1240./E_real(1)

1240./E_real(2)];

coeff=Mat^(-1)*Vec;Lnew=coeff(1)*L+coeff(2);Enew=1240./Lnew; % polynomial coefficients

end

if length(E_exp)==1

coeff=-E_exp(1)+E_real(1);Enew=E+coeff;

end

end

if n_pol==2 % polynomial degree =2: to be used with 3 spectral features

Mat=[(1240./E_exp(1))^2 1240./E_exp(1) 1

(1240./E_exp(2))^2 1240./E_exp(2) 1

(1240./E_exp(3))^2 1240./E_exp(3) 1]; % matrix Mat

Vec=[1240./E_real(1)

1240./E_real(2)

1240./E_real(3)];

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coeff=Mat^(-1)*Vec;Lnew=coeff(1).*L.*L+coeff(2).*L+coeff(3);Enew=1240./Lnew; % polynomial coefficients  
end
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