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Absolute energy calibration for plane grating monochromators

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Abstract

This report describes a new method for monochromator energy calibration, which is based on the freedom to change the fix focus constant c_{ff} in the plane grating monochromator at BESSY. If the monochromator is not perfectly aligned, spectra taken at different c_{ff}-values show energy shifts (of 1–2%). These can be attributed to offsets in the grating angles. Measuring spectra at different c_{ff}-values, one can determine these offsets by employing a fitting procedure. If these offsets are inserted, c_{ff} variation measurements lead to relative energy scale changes of less than a few 10^{-4}.

Keywords: Plane grating monochromators; Soft X-ray monochromator

1. Introduction

Monochromator energy scale calibrations are required for beamline commissioning work. Frequent rechecks during the lifetime of the monochromators are also necessary to correct for long term drifts of the storage ring or optical elements. Commonly, this work is accomplished by zero order checks and analysis of several known gas absorption spectra.

We report on a new method for monochromator energy calibration, which is based on the freedom to change the fix focus constant c_{ff} in the plane grating monochromator (PGM) at BESSY. If the monochromator is not perfectly aligned, spectra taken at different c_{ff}-values show energy shifts (of 1–2%). These can be attributed to offsets in the grating angles. Measuring spectra at different c_{ff}-values, one can determine these offsets by employing a fitting procedure. If these offsets are inserted, c_{ff} variation measurements lead to relative energy scale changes of less than a few 10^{-4}.

This method of absolute energy calibration has become possible due to the newly developed PGM generation [1], which not only allows for free variation of c_{ff}, but also contains in vacuum angu-lar encoders, which give high precision angular readings over a large angular range. Fig. 1.

2. Description of the calibration procedure

To calculate the true energy that is diffracted by the monochromator under angular offsets, one needs to consider the grating equation

$$Nk\lambda = 2\cos\Theta\sin(\Theta+\beta) \quad \text{and} \quad \Theta = \frac{\alpha+\beta}{2} \qquad (1)$$

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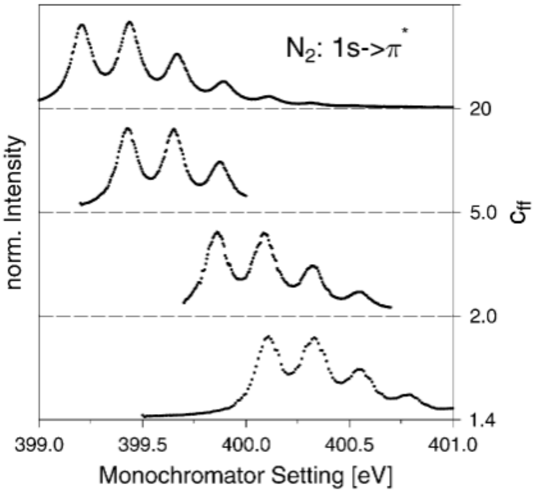

Fig. 1. N_2 gas absorption spectra, taken for different c_{ff}-values (right scale). The spectrum appears at different monochromator energies due to offsets in the grating angles (UE125-PGM at BESSY storage ring).

(N line density, k order of diffraction, λ wavelength, α incident angle, β diffraction angle), using [2]:

$$\sin\alpha = \left(\frac{\lambda Nk}{c_{ff}^2 - 1}\left(\sqrt{c_{ff}^2 + \frac{(c_{ff}^2-1)^2}{(\lambda Nk)^2}} - 1\right)\right)$$
$$\text{for } c_{ff} = \frac{\cos\beta}{\cos\alpha} \qquad (2)$$

and

$$\beta = -\arccos(c_{ff}\cos\alpha). \qquad (3)$$

Upon introduction of the grating (β) and plane mirror (Θ) errors: $\Delta\Theta$ and $\Delta\beta$, one observes the shifted wavelength

$$\lambda_s = \frac{2\cos(\Theta + \Delta\Theta)\sin(\Theta + \Delta\Theta + \beta + \Delta\beta)}{Nk}. \qquad (4)$$

This shifted wavelength, and therefore the shifted photon energy $E_s = hc/\lambda_2$ is a function of $\Delta\Theta$, $\Delta\beta$, and the true energy E.

Several simulated data are shown in Fig. 2 to illustrate the behavior of this function for different misalignments. There, it is nicely visible, that the β-offset is dominant for high c_{ff}-values. A real example of a N_2 absorption spectrum of the first peak in the $1s \to \pi^*$ resonance is shown as squares.

To find good estimates for $\Delta\Theta$, $\Delta\beta$, and E one has to perform a least squares fit to the shifted energy position. Here, the fitting gains significance if many c_{ff}-values are used and even higher orders are included. This is due to the fact, that larger angular ranges are explored. The latter, in turn, requires a good angular measurement. Fortunately, the BESSY plane grating monochromators contain in-vacuum angular encoders with a absolute accuracy of better than 2″ per 360° [3].

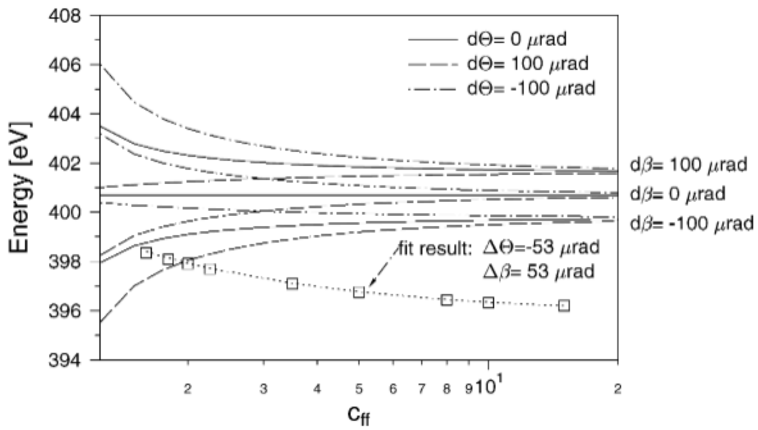

Fig. 2. Simulation of energy shift for different offsets. A real example (squares) is shown with the fitted result and corresponding corrections.

Table 1
N: groove density, $\Delta\Theta$, $\Delta\beta$ applied angular correction, E_{opt} energy found by fitting, ΔE remaining energy shift after correction

Beamline	N (l/mm)	Gas	$\Delta\Theta$ (mrad)	$\Delta\beta$ (mrad)	E_{opt} (eV)	ΔE (meV)
U125PGM	1200	N_2	0.105	0.240	400.77	290
	300	He	0.087	0.009	64.124	40
	1200	Ar	0.105	0.240	244.30	140
UE56/1-PGM	1200	N_2	−0.529	0.531	400.76	30
	1200	Ar	−0.518	0.518	244.29	20
	1200	Ne	−0.518	0.518	866.93	100
	1200	N_2	−0.064	−0.176	400.89	30
UE56/2-PGM-2	1200	Co	−0.168	−0.245	778.41	—
	1200	N_2	−0.093	0.106	400.71	25
	1200	N_2	−0.201	0.106	400.84	20
	400	N_2	−0.039	0.195	400.96	—
UE56/2-PGM-1	1200	N_2	0.029	0.405	400.66	130
	1200	N_2	−0.001	0.046	400.70	80
	400	N_2	−0.019	0.157	400.51	150

3. Examples

This calibration method has been used at BESSY on a longer term now. It has been counterchecked with the same measurements at different c_{ff}-values after applying the found angular corrections. In addition, zero order checks have been performed. All measurements indicate, that this procedure works very well for the BESSY PGMs. To give some idea of the quality of the calibration, many of the measurements are summarized in Table 1. In this table, one finds: the beamline at which the calibration was used, the gas that was used in the absorption cell, the line density of the grating, the fitted results of $\Delta\Theta$, $\Delta\beta$ and E, and the residual variation ΔE that was observed after applying the correction. The majority of the data shown gives residual errors of the order of 10^{-4}. Some calibrations are of less quality, which is probably due to variations in the electron beam position during the data acquisition.

4. Conclusion

The herein described energy calibration method has proven to be successful for the BESSY PGM-beamlines. It is a much quicker way of calibrating the energy axis than the classical method of measuring several gases and taking the zero order into account.

The energy scale checks after applying the fitted correction to the angles gives residual variations of the order of 10^{-4}. This is primarily due to the absolute angular encoders, used at the BESSY PGMs. In addition, these encoders ensure, that the calibration is not only valid at the measured energy, but for the whole energy scale, and even the zero order.

It is worth noting that the exact energy of the absorption feature, that is used for this analysis, needs not to be known. Therefore, this procedure can be used by the user of the beamline for unknown systems, even if the beamline is not properly calibrated. He simply has to acquire the apparent energy position of his feature at different c_{ff}-values. Subsequent fitting will reveal the true energy.

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