

# A SOFT X-RAY MONOCHROMATOR FOR THE UK NEW LIGHT SOURCE (NLS)

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## Abstract

The initial three FELs for the proposed UK NLS facility will cover the soft X-ray range 50 to 1000 eV in the fundamental and up to 5000 eV in the 3rd to 5th harmonics. Grating monochromators will be used for spectral filtering up to 2000 eV. This paper describes a flexible grating monochromator using a variable-included-angle plane-grating operating in collimated light that can operate in both pulse length preserving and high spectral resolving power modes. The performance of the monochromator operating over the fundamental range of NLS FEL-2 (250 to 850 eV) and the harmonics to 2000 eV is calculated.

## INTRODUCTION

The UK NLS is a free-electron laser facility that is intended to produce transform-limited pulses with a pulse length of 20 fs FWHM, giving a pulse bandwidth of  $\sim 0.09$  eV FWHM. These pulses can be used in many experiments without spectral conditioning. Some applications will, however, require spectral filtering of the pulses to 1) remove spectral content outside the main pulse bandwidth produced e.g. by SASE or spontaneous emission, or 2) improve the spectral resolving power from the inherent pulse bandwidth, or 3) remove the fundamental radiation when using the harmonics.

In the first and third scenarios, the inherent pulse length should be preserved as well as possible. This is problematic below 2000 eV where diffraction grating monochromators must be used. A diffraction grating works by creating a path length difference over the beam section of one wavelength times the order of diffraction for each illuminated groove. Thus, the grating acts to tilt the pulse-front in the longitudinal direction and this has the effect of temporally stretching the pulse. In normal synchrotron applications, this pulse stretch is negligible in the soft x-ray region, but it cannot be ignored with the short pulses from the NLS FELs.

The only way to absolutely preserve the pulse length whilst still using a grating to apply spectral filtering is to pass the pulse over a second grating so that the stretch created by the first grating is reversed [1]. The problem with this approach in the soft x-ray region is that the efficiency of gratings is rather low and so the overall transport efficiency of a double grating design will be poor ( $< 1\%$ ). This paper will describe how a single grating can be operated in such a way that the pulse stretch can be controlled so that it is similar to the input pulse length, whilst still giving high overall transport efficiency. Furthermore, the monochromator is flexible enough to also operate in a more conventional manner giving high spectral resolving power.

## PULSE LENGTH PRESERVATION

To describe how a grating monochromator can preserve the pulse length by introducing only a limited pulse stretch, we first note that the FEL source behaves as a near diffraction-limited Gaussian source. The RMS source size  $\sigma_r$  and the RMS source divergence  $\sigma_r'$  at a wavelength  $\lambda$  are thus related by (1):

$$\sigma_r \sigma_r' = M^2 \frac{\lambda}{4\pi} \quad (1)$$

where the  $M^2$  factor describes how far the source is from the diffraction limit. As the source will be longitudinally coherent, the RMS pulse length  $\Delta\tau_p$  and RMS energy bandwidth  $\Delta E_p$  in the pulse are related by (2):

$$\Delta\tau_p \Delta E_p = F \frac{h}{4\pi} \quad (2)$$

where  $F$  is a factor that defines how far from the Gaussian transform limit the pulse is. For a diffraction grating operating at an incidence angle  $\alpha$  (measured from the grating normal) and at a distance  $r$  from the source, the RMS illuminated length of the grating is given by (3) and the RMS pulse stretch from a grating of line density  $N$  in order of diffraction  $m$  is given by (4):

$$\sigma_L = \frac{r \sigma_r'}{\cos \alpha} \quad (3)$$

$$\Delta\tau_G = \frac{Nm\lambda\sigma_L}{c} \quad (4)$$

The RMS source-size limited energy resolution of the grating, determined by the angular subtend of the source at the grating, is given by (5):

$$\Delta E_s = \frac{hc}{Nm} \frac{\sigma_r \cos \alpha}{r \lambda^2} \quad (5)$$

By substituting the radiation divergence given by (1) into (3) and then substituting (3) into (4), we find that

$$\Delta\tau_G = \frac{M^2}{4\pi} \frac{Nmr\lambda^2}{c \sigma_r \cos \alpha} \quad (6)$$

Substitution of (5) into (6) gives

$$\Delta\tau_G = \frac{h}{4\pi} \frac{M^2}{\Delta E_S} \quad (7)$$

Expression (7) relates the pulse stretch caused by the grating to the source size limited resolution of the grating. If we set the source size limited resolution so that it is related to the pulse bandwidth by (8),

$$\Delta E_S = \frac{\Delta E_P}{F} \quad (8)$$

then from (2) we can see that the pulse stretch caused by the grating is related to the input pulse length by (9):

$$\Delta\tau_G = M^2 \Delta\tau_P \quad (9)$$

Thus, if the source is diffraction limited ( $M^2=1$ ), then by matching the grating resolution to the pulse bandwidth through (8), the pulse stretch will be equal to the input pulse length and the output pulse will be lengthened by a factor of just  $\sqrt{2}$ .

It is not a coincidence that the pulse stretch and grating resolution are related in this way. In the limit of an infinitely long grating in Gaussian illumination, the source size limited resolution is equal to the diffraction limited resolution as determined by the number of illuminated grooves. Since the pulse stretch is also determined by the number of illuminated groove, it is clear that in the case of pure Gaussian illumination from a transform-limited pulse, matching the source size resolution to the pulse bandwidth will also match the pulse stretch from the grating will to the length of the pulse.

This principal can be used to define the operating conditions under which a grating will give a stretch that is equal to (or some multiple of) the input pulse length. Combining (2), (5) and (8) gives:

$$\cos \alpha = \frac{Nm}{4\pi c} \frac{r}{\sigma_r} \frac{\lambda^2}{\Delta\tau_P} \quad (10)$$

If the grating stretch is desired to be less than the pulse length by a factor  $G$ , then the right hand side of (10) should be divided by  $G$ . The diffraction angle can be easily calculated from the grating equation.

$$Nm\lambda = \sin \alpha + \sin \beta \quad (11)$$

### Implementation of a PLP monochromator

To illustrate how the PLP (pulse length preserving) monochromator might work in practice, the case of a monochromator for FEL-2 of NLS is described. This FEL will operate in the fundamental from 250 to 850 eV in both linear and circular polarisation. Additionally, third and fifth harmonics will be available, though the grating beamline will only work to 2000 eV.

When working on the fundamental, the function of the monochromator will be to transmit only the transform limited spectral bandwidth of the pulse and thus remove wider spectral components created by SASE and spontaneous emission. When working on the harmonics, the main function will be to remove the fundamental radiation from the pulse.

Operating a grating with angles determined by (10) and (11) requires the included angle at the grating to be varied. This is best achieved with a plane grating monochromator of the SX700 type operating in collimated light [2]. The monochromator consists of a collimating mirror CM that collimates the light in the dispersive direction (hereafter assumed to be the vertical direction) followed by a plane mirror PM and a plane diffraction grating PG. Changing the incidence angle at the PM allows the included angle at the PG to be varied. The PM rotates about a point outside its surface and this allows a simple rotation to achieve the variation in included angle at the grating with only  $\mu\text{m}$  level motion of the beam along the grating over a relatively wide range of angles. After the PG a focussing mirror FM focuses the first diffracted order onto the exit slit. Because the grating operates in collimated light, the included angle can be freely chosen whilst still keeping the monochromatic focus at the slit. Indeed, the monochromator is essentially free from all aberrations in the dispersive direction provided the footprint on the FM is not too large.

It is clear from (10) that defining the operating parameters of the monochromator requires knowledge of the source. For this study it will be modelled as an ideal Gaussian TEM<sub>00</sub> source. The source size is taken to be 21  $\mu\text{m}$  RMS (a value suggested by early studies of the NLS FELs) and so the source divergence as a function of wavelength can be calculated from (1) with  $M^2=1$ . The pulse length is taken to be a constant 9 fs RMS and is perfectly transform limited, giving a bandwidth of  $\sim 0.09$  eV FWHM. The monochromator will be designed to add a pulse stretch equal to the inherent pulse length and thus the output pulse length will be  $\sim 13$  fs RMS.

In reality, of course, the source will not be so ideally behaved. The most important factor is how the source divergence deviates from the ideal (i.e. the value of  $M^2$ ) as this determines the illuminated footprint on the grating and hence the pulse stretch. The monochromator angles as a function of wavelength can either be adjusted to follow the actual source behaviour or the output pulse length can be allowed to deviate from the nominal value. Nevertheless, this idealised scenario will illustrate the how this monochromator concept functions.

The source to CM distance  $r$  must also be defined, and it has to be large enough to ensure the CM is not at risk of ablation by the FEL pulses. Calculations show that at a grazing angle of  $1^\circ$  with a Pt coating, the mirror should be at least 61 m from the source.

An important practical consideration is that the PM and PG grazing angles and lengths should be realistic. The off-axis rotation of the PM means that beam moves along it as the angle is varied and the PM length increases

dramatically as the grazing angle drops below  $\sim 1^\circ$ . Therefore, an angular offset of  $1^\circ$  between the input and the diffracted beams is introduced such that  $0.5^\circ$  is added to the PM grazing angle. The side effect of this is a negative impact on the monochromator efficiency.

The monochromator will work in first inside order of diffraction. Outside order operation reduces the footprint on the grating and so the pulse stretch, but this makes achieving high resolving power harder. In any case, in PLP operation, the grating operates close to zeroth order and so the gain from outside order operation is marginal.

Achieving low pulse stretch becomes increasingly difficult as the wavelength increases, mainly because each illuminated groove gives a bigger temporal stretch. Very low line densities must be used at the lowest photon energies and the entire energy range of the FEL must be covered with several gratings. Two gratings are needed to cover the fundamental range whilst a single grating can cover the harmonic range. The line densities chosen and the energy ranges are summarised in Table 1, which also gives the coatings of the PGs and PM. The PM will have longitudinal stripes of different coatings applied, which is practical since the sagittal beam footprint will only be  $\sim 1$  mm RMS. The CM and FM will operate at a fixed grazing angle of  $1^\circ$  with a Pt coatings to give good reflectivity from 250 to 2000 eV. It is advantageous if these mirrors deflect orthogonally to the dispersive plane (i.e. horizontally). Where SiC is required, an uncoated SiC substrate will be used; otherwise the substrate will be Si with a coating thickness of 400 Å.

Table 1: PLP Monochromator Parameters

Energy Range (eV)	250-500	425-850	800-2000
Line Density (l/mm)	25	50	200
Groove Profile	Trapezoidal with $10^\circ$ base angles		
Groove Width ( $\mu\text{m}$ )	21	11	3.2
Groove Depth (Å)	275	225	100
PG coating	Cr	SiC	Pt
PM coating	Ni	SiC	Pt
Grating angles at $E_{\min}$ ( $^\circ$ ) (inc. / diff <sup>n</sup> .)	3.02 / 3.15	2.09 / 2.31	2.36 / 2.76
Grating angles at $E_{\max}$ ( $^\circ$ ) (inc. / diff <sup>n</sup> .)	0.75 / 0.99	0.52 / 0.87	0.38 / 0.98

The grating angles given in Table 1 are the grazing angles of incidence and diffraction at the minimum and maximum energies of each grating. The 25 l/mm grating operates very close to zero order at the minimum energy. This should not be a significant problem since the FEL beam is highly collimated and so it is possible to separate the first order beam from the zeroth and higher orders, though the FM will have to be placed about 5 m from the grating to achieve this. In general, the lowest operating energy for any grating is determined by when the

diffracted order approaches the zeroth order. To work at lower energies requires either a lower line density or an increase in pulse stretch. Maintaining 9 fs of pulse stretch below  $\sim 200$  eV may not be possible with this approach.

The efficiency of the monochromator for horizontally linearly polarised light is presented in Figure 1. The efficiency for vertically linearly polarised light and the phase shift were also calculated. The difference in reflectivities and the phase shift are very small at all photon energies and the monochromator will preserve circularly polarised light with a calculated polarisation degree greater than 0.999. Mirror reflectivities were calculated using standard Fresnel formulae whilst the grating efficiencies were calculated with the Gradif code [3] using tabulated values of the optical constants [4,5]. The groove widths and depths given in Table 1 gave the most balanced grating efficiency over the range of operation. The grating profile was modelled as a trapezoidal with  $10^\circ$  base angles – a typical value that can be achieved with holographic ion-etched gratings.

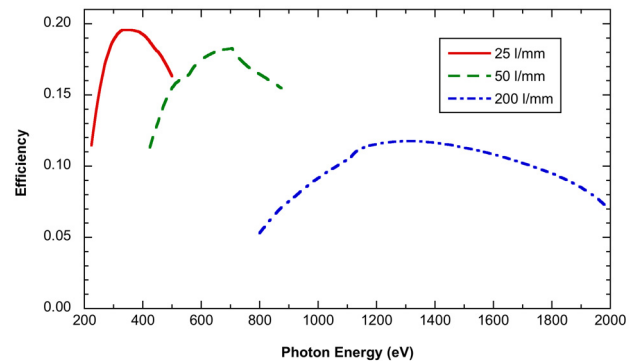


Figure 1: Monochromator efficiency in PLP mode.

The low line-density gratings help to give a very good overall efficiency throughout the range of the fundamental. A Cr coating on the PM for the 25 l/mm grating would give a very slightly higher efficiency but Ni has been used because it fits in better with the high resolving power operation (q.v.). The efficiency on the harmonics is less good but still very respectable for a soft x-ray monochromator. The grating actually gives an efficiency between 20% and 28%, but the rather high angles on the PM lead to give a reflectivity of only 45% at 800 eV. Covering the harmonic range with two gratings would improve the situation below 1300 eV considerably. For example, a 100 l/mm grating operating to 1300 eV would permit the SiC stripe on the PM to be employed which would double the PM reflectivity.

## HIGH SPECTRAL RESOLVING POWER

It is highly desirable for the monochromator to be able to work in a more conventional mode giving high spectral resolving power (HSRP). This gives greater flexibility for experiments by providing a more diverse range of photon probes, saves considerable cost by reducing the number of

day-one beamlines that have to be built, and preserves valuable floor space in the experimental hall for future beamlines. Since the monochromator has a free choice of included angle, this extra mode of operation is easy to implement. An 800 l/mm grating has been modelled over the fundamental range to illustrate possible performance. Coverage of the harmonics will not be required as they are expected to have ~0.09 eV bandwidth and so there is an inherently high resolving power above ~1000 eV. The monochromator will operate in the so-called “fixed-focus” mode where the incident and diffraction angles are related to the fixed-focus constant  $C_{ff}$  by (12). In this study  $C_{ff}=2.5$  has been used, but there is considerable scope to vary this and the line density depending on the resolving power (RP) required.

$$C_{ff} = \frac{\cos \beta}{\cos \alpha} \quad (12)$$

The monochromator can work over the entire range of the fundamental with a Pt coated PG in conjunction with the Pt stripe on the PM. However, the efficiency with Pt is not very high due to poor reflectivity of the PM (45 to 55%). This is the consequence of the increase in PM angle resulting from the angular offset of the input and diffracted beams that was required for the PLP operation.

In consequence, most of the fundamental range will be covered using a Ni coating on the PG and the PM. Furthermore, since the optimum groove depth naturally varies with photon energy, advantage will be taken of developments in grating manufacturing that allow the groove depth to be varied across the grating– the so-called VGD (varied groove depth) grating [6]. The monochromator parameters are summarised in Table 2.

Table 2: HSRP Monochromator Parameters

Energy Range (eV)	250-500	350-750	600-850
Line Density (l/mm)	800	800	800
Groove Profile	Trapezoidal with 10° base angles		
Groove Width (µm)	0.9	0.9	0.9
Groove Depth D (Å)	160	120	100
PG coating	Ni	Ni	Pt
PM coating	Ni	Ni	Pt
RP at $E_{min}$	46,000	39,000	30,000
RP at $E_{max}$	33,000	27,000	26,000

Figure 2 shows the calculated monochromator efficiencies. They are plotted over an extended energy range to illustrate the benefit of using the VGD grating. Using Ni gives a very good efficiency for a high RP monochromator and the VGD extends the upper photon energy before the switch to Pt must be made.

The expected resolving powers given in Table 2 have been predicted by vectorially summing the contributions

from the source size, a 10 µm exit slit at 20 m from the FM, and the slope errors of all the optics. The slope errors of the CM and FM have little effect on the resolution since they deflect orthogonal to the dispersive direction. However, the slope errors on the PM and PG are critical and limit the spectral resolving power. Challenging but achievable slope errors of 0.1 µrad RMS for the PG and 0.3 µrad RMS for the PM have been assumed.

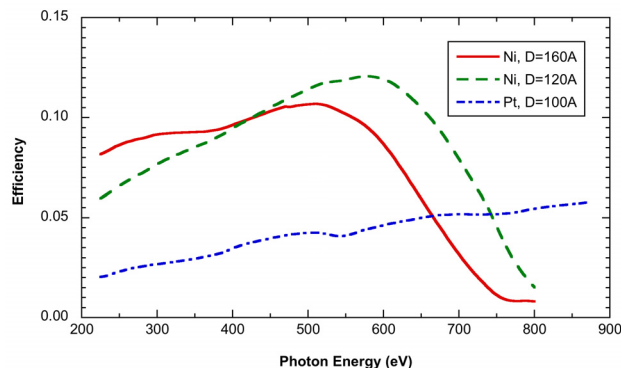


Figure 2: Monochromator efficiency in HSRP mode.

## CONCLUSION

This paper has shown that it is possible for a soft X-ray monochromator to work in different modes, giving either short pulses (~30 fs FWHM) or high spectral resolving power, with good overall efficiency in both modes.

It is easier to achieve low pulse stretch and high efficiency with a monochromator using gratings in the extreme-off-plane mount (conical diffraction). But then achieving high spectral resolving power would require extremely high line densities (> 8000 l/mm in this case) and efficiency would be poor.

The scheme proposed here is however not without technical challenges, mainly associated with making the very low line density gratings, and the minimum feasible pulse stretch increases as the photon energy decreases.

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