Grating Scatter due to Random Imperfections in the Grating Bar Shapes

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June 5, 1997

1 Introduction

Recent tests of the HEG gratings indicate that there is scattering along the dispersion direction near first order. This scatter can be the result of monochrometer leakage or by imperfections in the diffraction grating.

In this work, I show that the scattering observations are consistent with small ($\approx 2\%$) deviations of grating bar shapes from their ideal shapes.

2 Theory

Consider a diffraction grating composed of N lines with period d and a photon with wave number $k = 2\pi/\lambda$ incident upon the grating. It follows from Huygens principle that the *amplitude* for scattering by an angle θ with respect to the normal of the grating is given by[1]

$$I_N(k,s) = \frac{1}{N} \sum_{j=0}^{N-1} e^{ijksd} F_j(k,s), \tag{1}$$

where $s = \sin\theta$ and the *structure factor* $F_j(k,s)$ is defined by

$$F_j(k,s) = \frac{1}{d} \int_0^d \mathrm{d}x \; e^{iksx + i\phi_j(x)}. \tag{2}$$

The shape and composition of an individual grating element determines the phase shift $\phi_j(x)$. In general, $\phi_j(x)$ is a function that depends upon energy and, possibly, the polarization of the photon. Assuming the validity of scalar diffraction theory, the phase shift can be written in the form

$$\phi_j(x) = -k(\delta - i\beta) z_j(x), \tag{3}$$

[1] The factor $1/N$ has been introduced to make $|I_N(s,k)|^2$ evaluated at the points $s = n\lambda/d$ numerically equivalent to the grating efficiency. $|I_N(s,k)|^2$ can also be thought of as the average intensity per grating element.

where δ and β are energy dependent functions related to the dielectric constant of the grating bars. The function $z_j(x)$ represents the path length of the photon as it passes though the jth grating bar; it is sometimes called, rather loosely, the "grating bar shape", and more rigorously, the "path-length function".

In general, the structure factor $F_j(k,s)$ will vary with the grating bars because the "bar shape" will vary from bar to bar. Denote the average structure factor by

$$\bar{F}(k,s) = \langle F_j(k,s) \rangle \tag{4}$$

and define $f_j(k,s)$ to be the deviation of the jth bar from the mean via

$$F_j(k,s) = \bar{F}(k,s) + f_j(k,s). \tag{5}$$

Substituting the above definitions into (1) and taking the complex square to compute the intensity yields

$$|I_N|^2 = |\bar{F}|^2 \frac{\sin^2(\frac{Nksd}{2})}{N^2 \sin^2(\frac{ksd}{2})} + \frac{1}{N^2} \sum_{j,l} e^{iksd(j-l)} \langle f_j f_l^* \rangle. \tag{6}$$

For very large N, the first term goes to zero like $1/N^2$ except when ksd is a multiple of 2π where it becomes independent of N. For such values, one obtains the familiar grating equation

$$n\lambda = d \sin\theta. \tag{7}$$

Thus, the first term represents the familiar interference pattern that consists of a $1/N^2$ background with a series of sharp peaks whose height is $|\bar{F}(k,s)|^2$ and whose width vanishes as $1/N$. The second term is more complicated and appears to go to zero as $1/N^2$. However, as will be seen this is not necessarily true.

The quantites $\langle f_j f_l^* \rangle$ represent correlations between the various grating elements. If the shape of each grating element were independent of the others, then $\langle f_j f_l^* \rangle$ would vanish except when $j = l$. More explicitly, if no correlations are present,

$$\langle f_j f_l^* \rangle = \langle |f_j|^2 \rangle \delta_{jl}. \tag{8}$$

Assuming the absence of correlations and the reasonable assumption that $\langle |f_j|^2 \rangle$ is independent of j, the second term of (6) reduces to

$$\frac{1}{N} c_0^2(k,s) \tag{9}$$

where $\langle |f_j|^2 \rangle$ has been denoted by c_0^2.

In general $F_j(k,s)$, and hence $c_0(k,s)$, is a slowly varying function of s. This means that the intensity as a function of s will consist of sharp spikes at values of s satisfying the grating equation on top of a very weak but non-zero scattering continuum.

If there are correlations between the various grating bars, (8) is not correct. In general, we expect any correlations that may be present to have a short range. That is, it is reasonable to assume that $\langle f_j f_l^* \rangle$ is zero for $|j-l|$ greater than some number M. For example, if $M = 1$, then only nearest neighbor correlations may be present. If $M \ll N$, then one may neglect edge effects and write the scattering term in (6) as

$$\frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{m=-M}^{M} e^{imksd} \langle f_j f_{j+m}^* \rangle. \tag{10}$$

With the assumption that the grating is homogeneous on the scale set by the correlation length M, $\langle f_j f_{j+m}^* \rangle$ cannot depend on j and the scattering term reduces to

$$\frac{1}{N} \sum_{m=-M}^{M} e^{imksd} c_m(k,s) \tag{11}$$

where c_m has been defined by

$$c_m(k,s) = \langle f_j(k,s) f_{j+m}^*(k,s) \rangle. \tag{12}$$

Using the property that $c_{-m} = c_m^*$, which follows from the definition of c_m, and separating out real and imaginary parts, it follows that (6) may be written

$$|I_N|^2 = |\bar{F}|^2 \frac{\sin^2(\frac{Nksd}{2})}{N^2 \sin^2(\frac{ksd}{2})} + \frac{c_0^2}{N} + \frac{2}{N} \sum_{m=1}^{M} \left\{ \Re c_m \cos(mksd) + \Im c_m \sin(mksd) \right\} \tag{13}$$

The previous equation shows that the intensity pattern will consist of sharp diffraction peaks on top of a very weak but diffuse scattering background. The actual angular dependence of the diffuse scattering will depend upon the precise nature of the correlations and upon the correlation length given by M. Because of energy conservation, the scattering will reduce the height of the diffraction peaks. That is, the effectiveness of a grating whose bar shapes fluctuate will be lower than one that is perfect.

The fact that the scattering produced by the fluctuations in the grating bar shapes goes like $1/N$, whereas the sharp peaks of the diffraction pattern are on the order of unity, is somewhat misleading. In actual practice, the detector will have a finite angular acceptance and one ends up measuring the intensity integrated over some small angular region defined by the resolution of the detector (e.g., a pixel). Since the diffraction peaks have a width that scales like $1/N$, the integrated intensity will also go like[2] $1/N$. The end result is that the $1/N$ power of a diffraction peak is confined to a very tiny spatial region whereas the $1/N$ power of the scattering is smeared across a large region.

[2] One must not be alarmed by this result. The normalization employed here means that the intensity is for a *single* grating element.

One can make these comments more precise as follows. It is well known that the sequence of functions

$$2\pi\delta_N(x-a) = \frac{\sin\frac{1}{2}N(x-a)}{\frac{1}{2}(x-a)} \tag{14}$$

approaches the delta distribution as N goes to infinity. For very large N, $\delta_N(x-a)$ is very sharply peaked about the point $x = a$ with the height of the peak given by N. Using this function, the first term in (13) may be approximated by[3]

$$|\bar{F}(k,s)|^2 \cdot \frac{2\pi}{N}\delta_N(ksd - 2\pi n) \tag{15}$$

where n is an integer that denotes the diffraction order. Let Δs denote the angular resolution of the detector and define $s_n = 2\pi n/kd$. The probability that a photon will be detected at the position s with $s_n - \Delta s/2 <= s < s_n + \Delta s/2$ is proportional to

$$\int_{s_n-\Delta s/2}^{s_n+\Delta s/2} \mathrm{d}s\, |I_N(k,s)^2| \approx \frac{2\pi}{N}\frac{1}{kd}|\bar{F}(k,s_n)|^2 \tag{16}$$

where the contribution from the scattering terms in (13) has been neglected.

Outside this angular range away from a diffraction peak, $\delta_N(ksd - 2\pi n)$ is effectively zero and the scatter terms cannot be neglected. With the assumption that the correlation functions $c_m(k,s)$ do not vary much with s from pixel to pixel, the probability that a photon will scatter into an adjacent pixel is approximately proportional to

$$\frac{\Delta s}{N}\left\{ c_0^2(k,s_n) + 2\sum_{m=1}^{M} \Re c_m(k,s_n). \right\}. \tag{17}$$

As an example, suppose that the N grating bar shapes differ from one another only by a shift. That is, grating for the jth bar is assumed to be given by $z_j(x) = z(x + a_j)$ where a_j denotes the shift of the jth bar. Furthermore, assume that $z(x)$ is non-zero only for values of x such that $|a_j| <= x <= d - |a_j|$ for all j. Physically, this means that the center of the grating bar whose shape is described by $z(x)$ lies near middle of the grating element. Then, the structure constant F_j for the jth grating element can be written

$$\begin{aligned} F_j(k,s) &= \frac{1}{d}\int_0^d \mathrm{d}x\, e^{iksx+i\phi(x+a_j)} \\ &= \frac{1}{d}e^{-iksa_j}\int_{a_j}^{d+a_j} \mathrm{d}x\, e^{iksx+i\phi(x)} \\ &= \frac{1}{d}e^{-iksa_j}\left(\int_0^d + \int_d^{d+a_j} - \int_0^{a_j}\right)\mathrm{d}x\, e^{iksx+i\phi(x)} \end{aligned} \tag{18}$$

[3]Note that care has been taken to avoid the square of δ_N since it is well known that the square of a delta function is meaningless.

With the assumption that $z(x)$, and hence $\phi(x)$, vanishes for $x < |a_j|$ or for $x >= d - |a_j|$, the latter two integrations can be performed with the result

$$F_j(k,s) = e^{-iksa_j} F(k,s) + \frac{1}{iksd}(1 - e^{-iksa_j})(e^{iksd} - 1) \tag{19}$$

Here, $F(k,s)$ has been defined

$$F(k,s) = \frac{1}{d}\int_0^d \mathrm{d}x\; e^{iksx + i\phi(x)}. \tag{20}$$

From this, it trivally follows from (4), that

$$\bar{F}(k,s) = \langle e^{-iksa_j}\rangle F(k,s) + \frac{1}{iksd}(e^{iksd} - 1)(1 - \langle e^{-iksa_j}\rangle) \tag{21}$$

and we also deduce from (5) that

$$f_j(k,s) = \left[e^{-iksa_j} - \langle e^{-iksa_j}\rangle\right]\left[F(k,s) - \frac{1}{iksd}(e^{iksd} - 1)\right] \tag{22}$$

For values of $s = s_n$, these expressions reduce to

$$\bar{F}(k,s_n) = \langle e^{-i2\pi n a_j/d}\rangle F(k,s) \tag{23}$$

and

$$f_j(k,s_n) = (e^{-i2\pi n a_j/d} - \langle e^{-i2\pi n a_j/d}\rangle)F(k,s) \tag{24}$$

Thus this particular model of grating bar fluctuations produces no scattering in the immediate vicinity of zeroth order. The correlation function at $s = s_n$ reduces to

$$\langle f_j(k,s_n) f_l(k,s_n)\rangle = (\langle e^{-i2\pi n(a_j - a_l)/d}\rangle - \langle e^{-i2\pi n a_j/d}\rangle\langle e^{i2\pi n a_j/d}\rangle)|F(k,s_n)|^2. \tag{25}$$

Assume that the shift parameters a_j are independently gaussian distributed with a mean of 0 and a variance of σ^2. For such a distribution, one can show that

$$\langle e^{-i2\pi n a_j/d}\rangle = e^{-\frac{1}{2}(2\pi n\sigma/d)^2} \tag{26}$$

from which it follows

$$|\bar{F}(k,s_n)|^2 = |F(k,s)|^2 e^{-(2\pi n\sigma/d)^2} \tag{27}$$

and

$$c_m(k,s_n) = \delta_{m,0}|F(k,s)|^2(1 - e^{-(2\pi n\sigma/d)^2}). \tag{28}$$

Using these results together with (16) and (17) yields that the ratio of photons scattering in a region of size Δs around the nth order to those scattering into the nth order is roughly

$$\frac{kd\Delta s}{2\pi}[e^{(2\pi n\sigma/d)^2}-1] \approx 4\pi^2 n^3 \frac{\Delta s}{s_n}(\frac{\sigma}{d})^2. \tag{29}$$

We see that, for this particular model, the scattering becomes much more important for higher orders. Taking $\sigma/d \approx 0.025$ and Δs as one tenth of the dispersion distance s produces the estimate that the background in the vicinity of first order will consist of roughly 0.25 percent[4] of first order photons.

3 Numerical Simulations

In this section the results of several numerical simulations of (1) are presented. The numerical studies concentrated on grating consisting of 10000 rectangular grating bars that differ from one another by a small shift about their ideal lattice positions. The period of the grating was assumed to be 0.2 microns, the width was fixed at one half the period while the height was fixed at 0.7 microns.

For a rectangular lattice with uncorrelated gaussian shifts, (1) is exactly soluble allowing an independent check upon the numerical results. The calculations outlined in the previous section for this particular geometry are straightforward with the result

$$|I_N(k,s)|^2 = |\bar{F}(k,s)|^2 \frac{\sin^2(\frac{Nksd}{2})}{N^2\sin^2(\frac{ksd}{2})} + \frac{1}{N}c_0^2(k,s) \tag{30}$$

where

$$\begin{aligned} |\bar{F}(k,s)|^2 = \Big\{ & [\sin(\frac{ksd}{2}) - \sin(\frac{ksw}{2})]^2 \\ & + 2\sin(\frac{ksw}{2})[\sin(\frac{ksd}{2}) - \sin(\frac{ksw}{2})]e^{-kh\beta}\cos(kh\delta) \\ & + \sin^2(\frac{ksw}{2})e^{-2kh\beta}\Big\}\ (\frac{2}{ksd})^2 e^{-(ks\sigma/d)^2} \end{aligned} \tag{31}$$

and

$$c_0^2(k,s) = (1-e^{-(ks\sigma/d)^2})(\frac{2}{ksd}\sin(\frac{ksw}{2}))^2\Big\{1-2e^{-kh\beta}\cos(kh\delta)+e^{-2kh\beta}\Big\} \tag{32}$$

Here, w, h, and d are the bar width, bar height, and grating period, respectively, and σ is the standard deviation of the bar shifts.

4 Conclusion

[4]This result is consistent with the XRCF observation of first order photons at 1.775 KeV. See `http://space.mit.edu/HETG/xrcf_mysteries.html` for more information.