Diffraction efficiency of echelles working in extremely high orders

E. Loewen, D. Maystre, E. Popov, and L. Tsonev

A proposal to use a high-angle echelle in the vacuum UV in the 350th order triggered a theoretical study to determine if there were unusual obstacles to success. No serious obstacles were found except for efficiency limitations.

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An echelle with period $d = 22.71$ µm and an apex angle of 90° is investigated in the spectral region around wavelength $\lambda = 121.6$ nm. These unusual parameters were chosen to match desirable detector dimensions and lead to the interesting question of whether it is safe to design a spectrometer with an order of operation that far exceeds common limits. The grating material is considered to be bare aluminum and the surface to be completely smooth with no random roughness. The investigations were performed with a computer code based on the integral formalism for modeling light scattering by relief gratings. This is a rigorous method that takes into account Maxwell equations and vector boundary conditions without approximations. Approximations were introduced in the process of numerical solution where truncation of the infinite set of equations is necessary. Because of the very high period-to-wavelength ratio (almost 200), it was necessary to increase the truncation parameter so that the resulting matrices were dense matrices of the order of 1000–1500. A convergence with respect to the truncation parameter was obtained. Energy balance for a perfectly conducting substrate was used as an additional check of the validity of the results.1

We performed several different investigations, varying the wavelength and profile parameters. Both TE (or s or $P$) and TM (or $p$ or $S$) polarizations of light were studied. The TE vector polarization results are shown by solid curves and the TM ones by dotted curves. The figures give the spectral dependence of absolute efficiency (the ratio between the diffracted and incident power) in several consecutive orders. The direction $\theta_N$ of the diffracted order with number $N$ can be easily obtained from the grating equation,

$$\sin \theta_N = \frac{\lambda}{d} - \sin \theta_i,$$

(1)

where all the angles are measured from the grating normal and $\theta_i$ is the incident angle.

All the figures are shown in two layouts: The first is a general view and the second is with enhanced maximum resolution. The first investigation included a study of the diffraction efficiency of an echelle with an ideal triangular profile, working at an angle of incidence equal or close to the blaze angle $\varphi_B$, the angle of inclination of the small (active) facet. There are two sets of results: one set with a facet angle of 70° and one with a slightly different facet angle of 69.95° (the apex angle is always 90°). Assuming a constant angle of incidence of 70°, the spectral dependence of the diffraction efficiency in the 350th and 351st order are shown in Figs. 1 and 2. A shift of $\sim 0.04$ nm in the position of the maxima between Figs. 1 and 2 is observed. From the scalar theory expectations the position of the maximum $\lambda_B/\lambda$ is given by

$$\lambda_B = \frac{2d \sin \varphi_B}{N}.$$  

(2)

When the facet angle is changed from 70° to 69.95°, the expected shift of the 351st-order maximum is 0.039 nm, which corresponds to the one observed. However, because of the small width of the maxima, even this small shift results in an $\sim 2\%$ loss of efficiency [see Figs. 1(b) and 2(b)].
In addition to the shift in the maximum’s position caused by the blaze angle change, another shift can be detected: The maximum of the 351st order for a facet angle of 70° is observed at \( \lambda = 121.575 \) nm, whereas from Eq. (1) its position is determined at 121.598 nm. This deviation from the expectations of scalar theory result from the light scattering by a grating being an electromagnetic process. However, this shift corresponds to a variation in the facet angle of only 0.03°—an error much smaller than the technological ability to control it.

The other observation from the results of Figs. 1 and 2 is that the absolute efficiency can never exceed 80%, even theoretically and even for perfect profiles and the Littrow mount.

A second study was aimed at revealing the influence of departing from the Littrow mount, i.e., when the angle between the incident and the working diffraction order \( \text{[the angular deviation \{A.D.\] in-} \) increases, because in real devices the incident and the diffracted beams must be separated. In fact, Fig. 2(b) already shows that a small A.D. does not affect the maximum value; the shift of the observed wavelength and the change in the facet angle correspond to an A.D. at the maximum of the 351st order of 0.16°. However, in practice it is necessary to use higher A.D. values.

Figure 3 presents spectral dependencies of efficiency in 350th and 349th orders of the echelle with a 70° facet angle. Compared with Fig. 1, the difference is the angle of incidence, now assumed to be 75°, which ensures an A.D. of \( \sim 10° \) at 121.6 nm. There are two consequences: (1) The positions of the maxima are shifted. (2) Their values are diminished. According to scalar theory, a maximum in a certain order can be expected when this order is diffracted at the angle to which the incident wave is reflected from the active facet. We can easily deduce a simple equation, taking into account grating Eq. (1):

\[
\lambda_{\text{max}} = \lambda_B \cos \left( \frac{\text{A.D.}}{2} \right) .
\]

Fig. 1. Absolute efficiency of a 70° echelle used with a constant angle of incidence of 70° (close to the Littrow mount) on an aluminum surface. Orders as shown. Solid curve, TE polarization; dotted curve, TM polarization. (a) General view in the 120-nm spectral region; (b) scale expanded to show the order of the peaks.

Fig. 2. Same as Fig. 1 except the blaze angle is reduced from 70° to 69.95°.

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where $\lambda_{\text{max}}$ is the position of the maximum when A.D. is finite and $\lambda_B$ is as given by Eq. (2).

The correspondence between the real position of the maximum and the scalar prediction [Eq. (3)] is good. For example, the 350th-order maximum is observed at $\lambda = 121.474$ nm. Its diffraction angle then is equal to $64.985^\circ$, giving A.D. = 10.015°. The evaluated blaze wavelength at A.D. = 0° from Eq. (2) is 121.945 nm, so that the expected position of $\lambda_{\text{max}}$ from Eq. (3) is 121.480 nm, a difference that is negligible.

The position of the maximum differs from the desired one (121.6 nm), but when the angular devi-
Fig. 6. Same as Fig. 3 except the profile is deformed as in profile 4 in Fig. 5.

Fig. 7. Same as Fig. 3 except the profile is deformed as in profile 6 in Fig. 5.

Fig. 8. Same as Fig. 3 except the profile is deformed as in profile 5 of Fig. 5.
tion is varied slightly, it can be moved to the good position without the facet angle changing. If all the grating parameters are preserved, Eq. (3) predicts that for A.D. = 8.62° the maximum of the 350th order would be centered at 121.6 nm. The corresponding A.D. for the 349th order is 12.22°.

The numerical experiment (third study) shows a slight shift from the scalar predictions. Fixing the facet angle to 70°, we observe the maximum efficiency in the 350th order at λ = 121.6 nm when the angular deviation is 8.25° [Figs. 4(a) and 4(b)].

The next set of calculations (the fourth study) shows the influence of possible profile deformations on efficiency. Three different deformations were studied; their corresponding profiles are shown in Fig. 5. The deformations include a cut at the groove bottom, which is close to the experimental observations of several echelles. In profiles 4 and 6 the active facet is cut into two straight segments, with the efficiency shown in Figs. 6 and 7. The larger segment is inclined at 70° with respect to the grating plane, and the apex angle is kept at 90°. The height of the deformed segment for profile 4 is 0.8 µm, and for profile 6 it is 1.17 µm. Profile 5 resembles profile 6, but the small facet has a convex shape with the maximum deviation from the straight line 4 nm, as the results in Fig. 8 show.

The efficiency of profile 4 does not differ noticeably from the ideal profile [Fig. 3], whereas for profiles 5 and 6 there is a slight shift of the maximum and an ~1% decrease in efficiency, when compared with Fig. 3. The difference between profiles 5 and 6 is negligible.

The conclusions are as follows:

1. The efficiency is almost independent of the polarization.
2. There is a slight shift between the real position of the spectral maxima and those predicted from the scalar theory. This shift could be measured, as long as efficiency changes by several percent, but the results are masked by the uncertainty in knowing the true facet angle and the true profile form.
3. Even in the Littrow mount with an A.D. of 0° the absolute theoretical efficiency does not exceed 80%.
4. The angular deviation from the Littrow mount leads to a decrease in efficiency. For A.D. = 10° the decrease exceeds 24% but that improves with a reduced A.D.: An A.D. of 8.25° provides a theoretical peak efficiency of ~60%.

References