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Convergence of Rayleigh–Fourier method and rigorous differential method for relief diffraction gratings—non-sinusoidal profile

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Abstract. Influence of the grating profile on the convergence rates of the Rayleigh–Fourier and rigorous electromagnetic methods is illustrated. On increasing the number of Fourier components and or the asymmetry of the grating profile, the convergence of the Rayleigh–Fourier method drops off rapidly; while the results of the rigorous method are not substantially affected.

Although the Rayleigh method [1] is non-rigorous in a mathematical sense [2], Wirgin [3, 4] has shown that its Rayleigh–Fourier (RF) modification gives accurate results for sinusoidal gratings when the ratio of groove depth h to period d is five times greater than the theoretical value $h/d=0{\cdot}142$ [2]. The comparison between the convergence rates of the RF method and the rigorous differential method of Chandezon *et al.* [5] (C method) made in [6] confirms the conclusions of Wirgin for sinusoidal gratings. For deeper and/or coated gratings, however, the C method is more powerful [6]. Moreover, in the conical diffraction mounting the convergence of the numerical code of the generalized C method [7] remains practically the same as that for the in-plane case.

However, except for some holographic gratings, more often than not the actual grating profiles differ from the sinusoidal one. It is therefore important to know the possibilities of the different methods for investigation of gratings with arbitrary profiles. Hugonin *et al.* [8] have shown that the RF method provides reliable results only for sufficiently shallow triangular gratings.

In this paper, we compare the results of the approximate RF method and the rigorous C method for aluminium gratings with four different types of profile but only one h/d ratio.

The first example corresponds to a sinusoidal aluminium grating ($n_{\mathrm{Al}}=1{\cdot}23+\mathrm{i}\,6{\cdot}95$, $h=0{\cdot}2\,\mu$m, $d=0{\cdot}6\,\mu$m) illuminated by a TE polarized wave of wavelength $0{\cdot}6\,\mu$m in a Littrow mount. Figure 1 shows the efficiency calculated by the two methods as a function of the truncation parameter N [6], representing the number of the diffraction orders m, taken into account that $-N\leqslant m\leqslant N$. Contrary to [6], here we have not employed special subroutines for Bessel function calculations, but rather a simple trapezium-rule integration using 40 points per period of the profile function, which is applicable in the case of non-sinusoidal profiles as well. It appears that the convergence of both the methods has not been influenced by this approximation and, in particular, coincides with the convergence rates for a dielectric grating with the same h/d ratio (figure 7 of [6]).

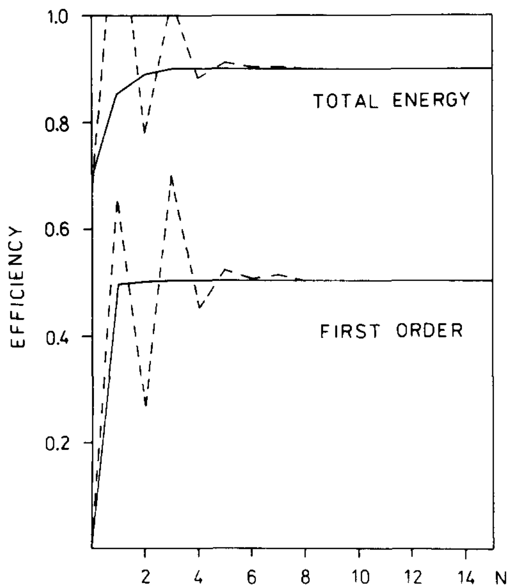

Figure 1. Convergence rates of the RF method (dashed line) and the C method (soli for a sinusoidal grating of aluminium coating.

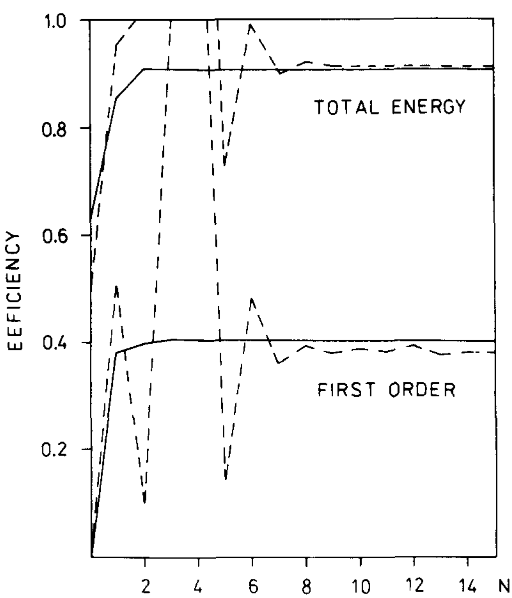

Figure 2. Same as in figure 1, except for a symmetrical triangular grating.

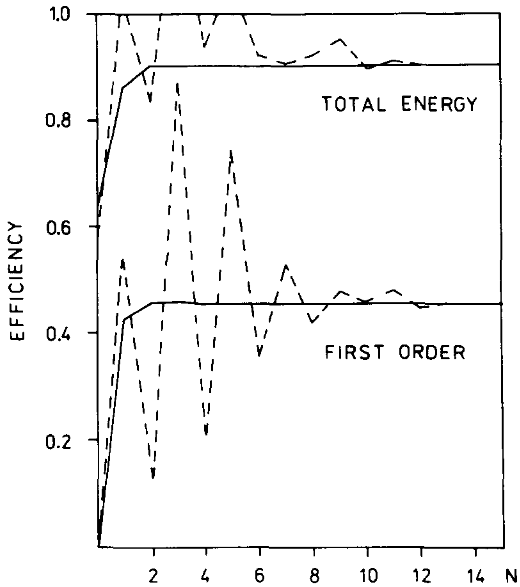

Figure 3. Same as in figure 1, except for the grating profile function represented by equation (2).

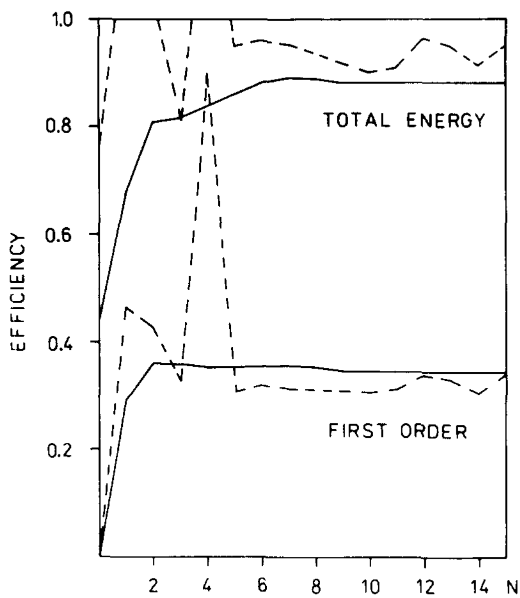

Figure 4. Same as in figure 1, except for an asymmetrical triangular grating with a blazed angle 21·8° and an apex angle 94·8°.

As a second example we considered a symmetrical triangular grating whose profile function can be expanded as a Fourier series:

$$f(x)=\frac{4h}{\pi^2}\sum_{m=0}^{\infty}(-1)^m\sin[(2m+1)2\pi x/d]/(2m+1)^2. \qquad (1)$$

The convergence rate (see figure 2) of the rigorous method is practically unaffected by the profile change, while the effect on the convergence of the RF method is affected drastically. For small N, the results of the RF method become highly oscillatory. On increasing the truncation parameter, the results do not reach stabilized values and, for example, for $N=20$ the deviation in the first order reaches 5 per cent. This can be understood by taking into account the existence of edges, which affect the validity of the Rayleigh hypothesis (see, for example, [9]) even for shallow gratings.

The efficiency of the grating with an interstitial between the triangular and sinusoidal profile is presented in figure 3. The profile function contains only the first two terms of (1):

$$f(x)=\frac{9h}{20}\left(\sin\frac{2\pi x}{d}-\frac{1}{9}\sin\frac{6\pi x}{d}\right). \qquad (2)$$

The normalization coefficients in (1) and (2) are chosen such that $\max f(x)-\min f(x)=h$. Even a slight deviation from a sinusoidal profile results in a great deterioration in the convergence of the RF method, while the C method provides accurate results even for small values of N.

The asymmetry of the grating profile amplifies the oscillations of the RF method (figure 4). The convergence of the rigorous method is slightly reduced, but a saturation value is reached, again for relatively small values of N.

In conclusion, for non-sinusoidal gratings, the approximate RF method has to be used most carefully. It seems that the number of the Fourier components and the asymmetry of the grating profile function are the main factors (in fact they are not independent) affecting the convergence of the RF method. The existence of edges, as expected, leads to a divergence of the result. On the other hand, the rigorous method gives reliable and rapidly converging values of the efficiency.

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