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# Gratings—general properties of the Littrow mounting and energy flow distribution

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**Abstract.** Quasi-periodicity under certain conditions of the dependence of grating properties on groove depth is explained from the point of view of energy flow distribution (EFD). The formation of curls in flow maps is followed as a function of the groove depth $h$ for two general types of gratings having one or two propagating diffraction orders. An equivalence between shallow and deep gratings is established: the EFD above the grooves is one and the same, while in deep gratings a definite number of curls exists, totally hidden inside each groove. Perfect blazing and antiblazing are connected with the position of these curls with respect to the top of the grooves.

## 1. Introduction

It is well known that gratings exhibit quasi-periodicity of properties when groove depth is varied. A detailed discussion can be found in reference [1], where a phenomenological approach is developed to study this effect. Numerical investigations [2] for very deep metallic gratings (groove depth to period ratio $h/d$ exceeding 6) supporting two propagating diffraction orders confirm the existence of such a quasi-periodicity. A typical example of this property can be found in figure 1: starting from a flat surface, more and more energy is diffracted into the $-1$st diffraction order as $h$ is increased; when $h/d \approx 0{\cdot}4$ (for TM polarization) almost all of the incident energy is diffracted—this is the so-called 'perfect blazing' in a Littrow mounting (accompanied, of course, by a zero of the 0th reflected order efficiency). Further increase of $h$ leads to a decrease of $\eta_{-1}$ (efficiency of $-1$st order). As $h/d \approx 0{\cdot}72$, the grating acts like a flat surface—all of the incident energy is specularly reflected. Moreover, this equivalence is valid not only in Littrow mounting, but for almost the entire interval of angles of incidence (the so-called 'antiblazing' of gratings [3]). As the groove depth increases further, the properties in the far-field zone change quasi-periodically.

In a subsequent paper [4] it is shown that if a surface plasmon is excited on a grating with a period that provides one diffraction order, its radiation losses (and all its other characteristics) are also quasi-periodical with $h$. Thus two obvious questions arise: namely how can these general macroscopic properties of gratings be

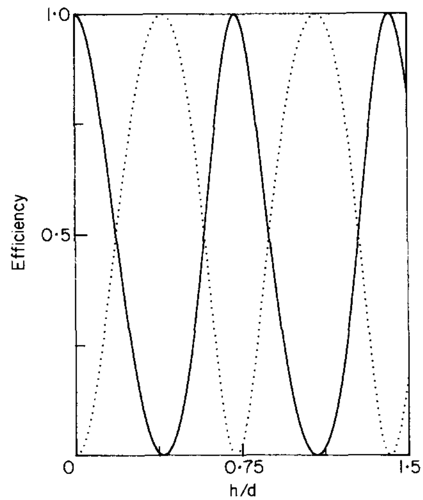



Figure 1. Diffraction efficiency of the 0th (solid line) and the −1st (dotted line) reflected order against groove depth to period ratio in the Littrow mounting for a perfectly conducting grating of period $d = 0{\cdot}5\,\mu\text{m}$ at wavelength $0{\cdot}6328\,\mu\text{m}$: sinusoidal profile.

interpreted? and what is the microscopic field structure that gives rise to such behaviour?

It is the aim of this paper to connect the phenomenon of quasi-periodicity of grating properties as a function of groove depth with peculiarities of energy flow distribution (EFD) and with the existence of curls in EFD in particular. For example, when antiblazing occurs, EFD above the grooves of deep gratings is the same as that above a flat surface, while inside each groove a definite (one, two, ...) number of totally hidden curls exist, separating the groove bottom from the flow in the upper space. The results presented in the next two sections are valid for perfectly conducting gratings. Perfect conductivity is not a limitation of the numerical method [5], but an important condition for visualizing EFD: not to have flow lines which finish on the metal surface. Nevertheless, it must be pointed out that the results (existence and formation of curls) are not restricted to perfect conductivity, this is shown in the subsequent paper [4]. The vacuum light wavelength is assumed to be $0{\cdot}6328\,\mu\text{m}$ throughout the present paper.

The second section of this paper includes results for a grating supporting two propagating diffraction orders (0th and −1st). The Littrow mounting condition implies an angle of incidence $\theta = \arcsin 0{\cdot}6328$ for a groove spacing of $0{\cdot}5\,\mu\text{m}$.

In the third section we deal with a grating supporting only a single specular diffraction order (0th) and having a period of $0{\cdot}3\,\mu\text{m}$. The angle of incidence $\theta$ satisfies the relation $\sin\theta = 0{\cdot}6328$. In this case there is a periodicity of the phase rather than the amplitude of the reflected wave. This case is interesting because curls are formed only in the near-field zone, while the far-field picture is identical to the EFD above a perfectly conducting flat mirror.

## 2. Grating supporting two diffraction orders

Further on we deal with figures representing the energy flow lines which are locally tangential to the Poynting vector **S** defined as

$$\mathbf{S}=\mathrm{Re}\,(\mathbf{E}\times\mathbf{H}^*), \tag{1}$$

where the asterisk means complex conjugation. The calculations were performed using a computer code based on the rigorous differential formalism of Chandezon *et al.* [2], which proved to be very efficient [5] for determining the electromagnetic field in both the far-field and near-field zones [6].

In the far-field zone the component of the electromagnetic field parallel to the grooves can be represented as a sum of incident, reflected and diffracted orders. For TM polarization this is the $z$ component of the magnetic field:

$$H=a_\mathrm{i}\exp[\mathrm{i}k(\alpha x-\chi y)]+a_\mathrm{r}\exp[\mathrm{i}k(\alpha x+\chi y)]+a_\mathrm{d}\exp[-\mathrm{i}k(\alpha x-\chi y)], \tag{2}$$

where $k=2\pi/\lambda$, $\alpha=\sin\theta$, $\chi=\cos\theta$ and $a_{\mathrm{i,r,d}}$ are the amplitudes of incident, reflected and diffracted components respectively. In equation (2), the $x$ axis is perpendicular to the grooves and lies in the grating plane and the $y$ axis is perpendicular to the grating plane. We are dealing with $-1$st order Littrow mounting in which the $-1$st diffraction order and the incident wave are propagating in opposite directions.

When the grating reduces to a perfectly conducting plane mirror located on the $x$ axis, $a_\mathrm{d}=0$ and $a_\mathrm{r}=a_\mathrm{i}$. Further on we assume that $a_\mathrm{i}\equiv 1$. Then it can easily be shown that the $x$ and $y$ components of **S** are given by

$$S_x=\frac{2ka}{\omega\varepsilon_0 n^2}[|a_\mathrm{r}|^2+Re\,(a_\mathrm{r})\cos(2k\chi y)], \tag{3}$$

$$S_y=\frac{2k\chi}{\omega\varepsilon_0 n^2}[\mathrm{Re}\,(a_\mathrm{r}a_\mathrm{d}^*)\cos(2k\alpha x)-\mathrm{Im}\,(a_\mathrm{r}a_\mathrm{d}^*)\sin(2k\alpha x)], \tag{4}$$

where $n$ is the refractive index of the upper lossless medium (assumed to be equal to unity), $\omega=c/k$, $c$ is the light velocity in vacuum and $\varepsilon_0$ vacuum permittivity. For example, (3) and (4) are greatly simplified if we assume that amplitudes $a_\mathrm{r}$ and $a_\mathrm{d}$ are real, (this is almost true for shallow gratings). When the profile function $f(x)$ is chosen such that the origin of the coordinate system always lies on the surface, for example if $f(x)=(h/2)\sin(2\pi x/d)$, then:

$$S_x=\frac{2k\alpha}{\omega\varepsilon_0 n^2}a_\mathrm{r}[a_\mathrm{r}+\cos(2k\chi y)], \tag{3 a}$$

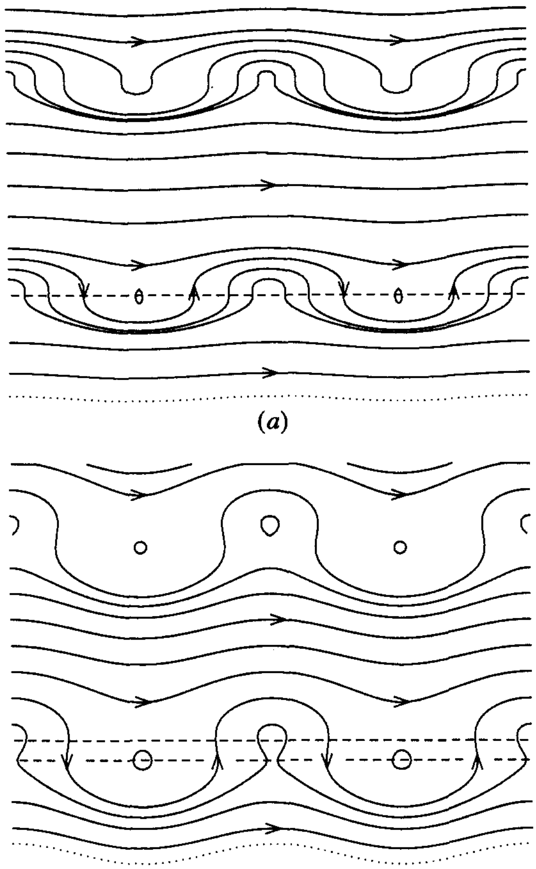
$$S_y=\frac{2k\chi}{\omega\varepsilon_0 n^2}a_\mathrm{r}a_\mathrm{d}\cos(2k\alpha x). \tag{4 a}$$

### 2.1. *Shallow gratings*

#### 2.1.1. *Flat surface*

In the well known case of a flat surface the vertical ($S_y$) component of the Poynting vector becomes zero, as $a_\mathrm{d}=0$. This case is characterized by flow lines parallel to the surface, (there are no losses in either medium). For TM polarization $S_x$ has a maximum on the surface ($y=0$), and has a zero at a height

$$y_0^{\mathrm{TM}}=(2m+1)\frac{\pi}{2k\chi},\quad m=0,1,\ldots. \tag{5 a}$$



(a)

(b)

Figure 2. Energy-flow distribution above the surface of the grating described in figure 1: shallow gratings. In (a) $h/d=0{\cdot}02$; in (b) $h/d=0{\cdot}08$.

For TE polarization $S_x$ is zero at the surface and when

$$y_0^{\mathrm{TE}} = 2m\frac{\pi}{2k\chi}, \tag{5b}$$

and has a maximum where $S_x^{\mathrm{TM}}$ exhibits zeros.

### 2.1.2. *Shallow gratings*

As the groove depth becomes slightly greater than zero, the diffracted field amplitude becomes non-zero also. As there is no absorption in either medium, in the very near vicinity of the grating the flow lines must follow the groove profile without osculating the surface (figure 2 (a)) and curvature of the lines is apparent. Indeed, equation (4 a) states that $S_y \not\equiv 0$ except for the vertical lines above the tops and bottoms of the grooves (the profile is defined by the equation $y=(h/2)\sin(2\pi x/d)$): in the Littrow mounting $2\alpha=\lambda/d$ and $S_y=0$ for $x=(2m+1)d/2$. As now $|a_r|<1$, each horizontal line at which $S_x=0$ (equation 3 (a)) is split into two lines (figure 2 (b)), the splitting increases as $|a_r|$ decreases (i.e. with the increase of groove depth). Between each two pairs of lines $S_x$ has an opposite sign in comparison to the flat surface case. Two dashed lines in figure 2 (*b*) correspond to the splitting of the dashed line of figure 2 (*a*) and represent the positions where $S_x$ becomes zero. As a result of this changing of directions of $\mathbf{S}$, curls are formed around the points where $|\mathbf{S}|=0$. They exist even for very shallow gratings and wherever three waves are found to be interfering, there will be regions where curls exist. It is shown in [7] that the interaction of three monochromatic circularly polarized electromagnetic waves can lead to very interesting physical phenomena and field distributions. It can easily be shown from (3 *a*) and (4 *a*) that curls are formed all over the area, independently of the origin of the three waves in (2). These waves can be the result of light diffraction from a grating, but could also be radiated by three different sources.

Returning to the grating, it must be pointed out that two different sets of curls are found (figure 2 (*b*)): above the tops (labelled further as top curls) and above the bottoms (labelled further as bottom curls) of the grooves, the second lying a little lower than the first. By increasing the groove depth the centres of the two sets of curls are shifted in a vertical direction and the curls are enlarged, thus enveloping more and more flow lines.

An important point must be made here: for TE polarization the formation of the lowest curls begins at twice the distance from the grating surface than in the TM case. This is a direct consequence of equation (5).

### 2.2. *Deep gratings*

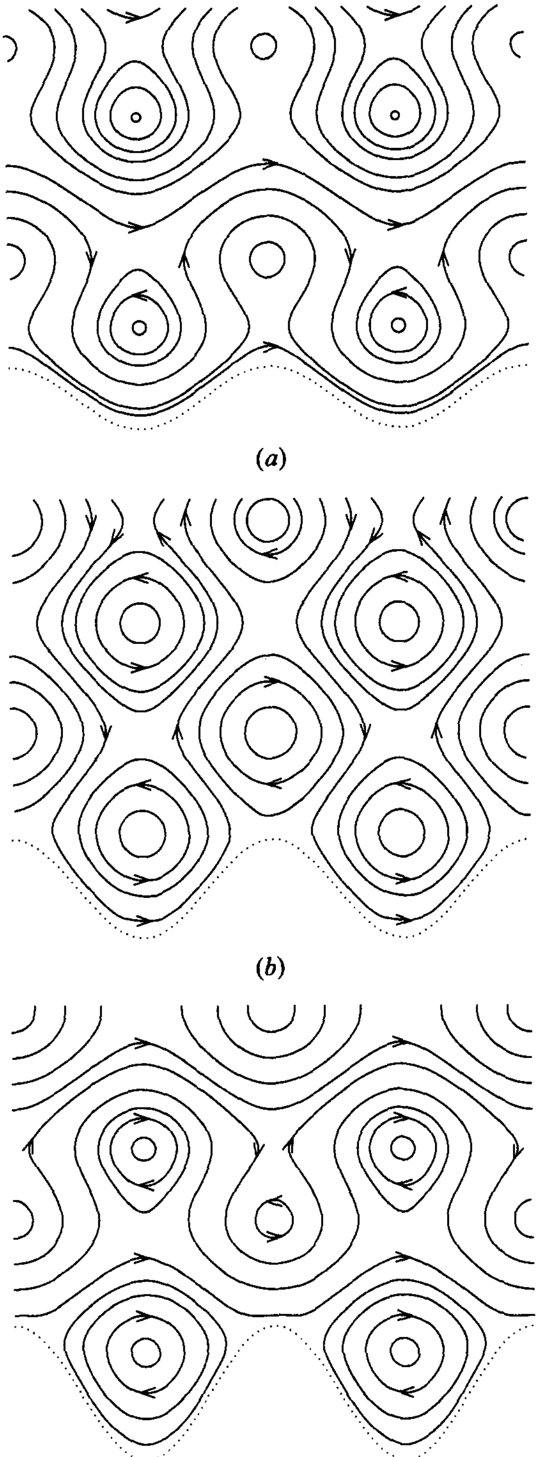
#### 2.2.1. *Perfect blazing in Littrow mount*

An increase of curls means that fewer and fewer flow lines pass from the left to the right (i.e. less energy is carried towards the positive direction of the $x$ axis (figure 3 (*a*))). As a consequence the amplitude of the reflected order $a_r$ decreases, and an increase of diffraction efficiency is observed. It is interesting to note that the centres of the lowest top curls and of the lowest bottom curls lie at almost the same height from the grating surface. Hence when $h$ is increasing, the vertical distance between the centres of the different sets of curls grows almost in proportion to $h$. When the centres of the lowest bottom curls fall on the line connecting the groove tops (figure 3 (*b*)), all the curls become uniformly spread, (the centres of the top curls are localized in a vertical direction exactly between the centres of the bottom curls). The curls then occupy the entire upper medium and no energy flow towards $+x$ is observed, thus $a_r=0$ and perfect blazing occurs. It can easily be predicted that this should happen when

$$h=y_0^{\mathrm{TM,TE}}. \tag{6}$$

Equation (6) is only a good approximation as to how far the evanescent waves are included in the near-field zone. However, it must be pointed out that although the grating becomes deeper and deeper, far-field and near-field EFD are identical except in the region of the groove, where the picture should depend on the form of the profile.

Equations (5) and (6) explain why TE perfect blazing can usually be obtained at approximately double the grating depth for TM polarization: the lowest curls are formed at surfaces of twice the height for TE polarization and groove depths of twice



(a)

(b)

(c)

Figure 3. Same as for figure 2, but for deep gratings. In (a) $h/d=0{\cdot}24$; in (b) $h/d=0{\cdot}38$; in (c) $h/d=0{\cdot}52$.

(a)

(b)

(c)

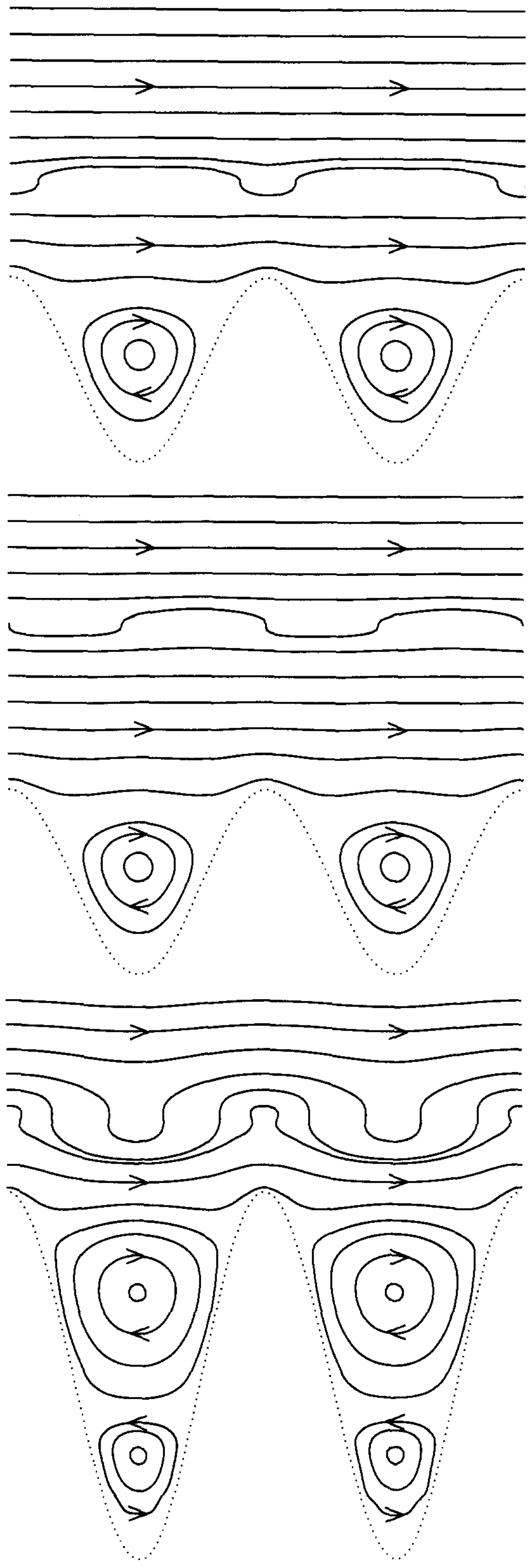


Figure 4. Same as for figure 2, but for very deep gratings. Figure 4 (*b*) is not in the Littrow mounting ($\sin\theta = 0{\cdot}6328$), but at $\theta = \arcsin(0{\cdot}85)$. In (*a*) $h/d = 0{\cdot}72$; in (*b*) $h/d = 0{\cdot}72$; in (*c*) $h/d = 1{\cdot}44$.

the height are required to bring the centre of the lowest bottom curls to the line connecting the tops.

When $a_r = 0$ it can easily be shown that not only are all the flow lines closed curves (figure 3 (*b*)), but $|\mathbf{S}|$ vanishes from the upper medium. As $h$ increases, the curls appear again, but now the rotation has an opposite direction. The bottom curls are lowered further with $h$ (figure 3 (*c*)). The increasing asymmetry in the position of the two sets of curls leads to a decrease in the area occupied by them. Thus more and more energy lines move from left to right and $a_r$ increases.

### 2.2.2. *'Antiblazing' of gratings*

The curls continue to unfold as the lowest bottom curls occur deeper in the grooves as the groove depth increases. The vertical distance between the centres of the second bottom curls and the first top curls decrease and, except in the groove region, the EFD increasingly resembles the EFD of shallow gratings. When the centres of both sets of curls occur on one horizontal line, the EFD above the grooves is the same as above a plane surface. Then the first (i.e. lowest) bottom curls totally separate the flow above the grooves from the groove surfaces (figure 4 (*a*)). They are therefore deformed in such a way as to wind the profile.

Since the EFD is the same as above a flat surface, no diffraction is observed ($a_d = 0$). The curls inside the grooves are very stable and feel practically no influence from the angle of incidence (figure 4 (*b*) with $\alpha = 0{\cdot}85$). Thus the so-called 'antiblazing' of gratings [3]—when $-1$st order efficiency is zero in the Littrow mounting it is almost zero everywhere—finds its physical interpretation.

### 2.3. *Very deep gratings*

Further increase of $h$ leads to a repetition of the EFD for shallow gratings, except for the existence of a hidden curl inside each groove. These curls occur lower and lower inside the grooves as $h$ increases. In the case of a very deep groove, a second perfect blazing occurs ($h/d = 1{\cdot}08$ of figure 1), followed by a second 'antiblazing'. The latter is characterized by two hidden curls inside each groove that separate the flow above the grooves from that at the bottom (figure 4 (*c*)).

## 3. Grating supporting a single diffraction order

A natural question arises in connection with the results of the previous section: as far as the properties of the two-diffraction-order gratings can be interpreted in terms of formation of curls (and these curls are formed all over the upper medium), what is the EFD in the near-field zone of a grating supporting only one diffraction order? We know that the far-field picture is equivalent to the distribution over a flat surface as far as we have assumed perfect conductivity. In that case there is again a quasiperiodicity of the grating properties even in the far-field zone, but with respect to the phase, rather than the amplitude of the reflected wave (figure 5). Representations of EFD above a perfectly conducting grating with period $d = 0{\cdot}3\,\mu m$ are presented in figures 6 (*a*)–(*c*) for groove depth values corresponding to some important regions of figure 5. Again, formation of curls is observed, but now only in the near-field zone (figure 6 (*a*)). They are formed again on the line corresponding to

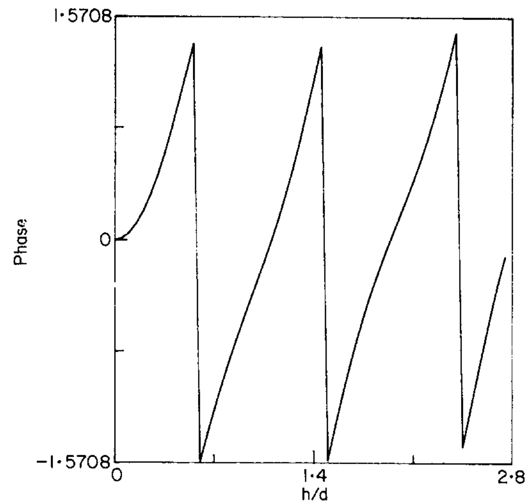



Figure 5. Phase of the 0th reflected order against groove depth to period ratio for a perfectly conducting grating of period $d = 0{\cdot}3\,\mu m$ at wavelength $0{\cdot}6328\,\mu m$: sinusoidal profile. Angle of incidence $\theta = \arcsin(0{\cdot}6328)$.

$|\mathbf{S}| = 0$ for a plane surface. The main differences from the case of $d = 0{\cdot}5\,\mu m$ (figure 2 (*a*)) are:

(1) The curls are formed only in the near-field zone. Going away from the grating they become smaller and smaller and when evanescent diffraction orders vanish, EFD becomes the same as that above a flat surface.

(2) The bottom curls are formed higher than the top curls. Thus, when $h$ increases further, the top curls are unfolded. This last peculiarity has a direct consequence: energy flow for shallow gratings in the very near vicinity of the surface has the opposite direction to that of the far-field flow.

Further increase of $h$ moves the lowest bottom curls deeper into the grooves. At a certain value of $h$ such curls are totally hidden (figure 6 (*b*)). This corresponds to the zero phase difference between waves reflected by the grating and by a flat mirror. In this case the EFD above the grooves is identical with the EFD above the flat surface, as may be anticipated by considering the results of the previous section. Further increase of groove depth results in the same effect upon the EFD as that induced by shallow gratings, except that inside each groove one curl goes deeper and deeper. Figure 6 (*c*) presents EFD corresponding to the second point of figure 5 with zero phase difference ($h = 0{\cdot}58\,\mu m$). Again, above the grooves the EFD resembles the flat surface case, but now two curls are hidden inside each groove.

## 4. Conclusion

Visualizing the EFD above and inside the grooves of shallow, deep and very deep gratings enables us to find new and useful physical interpretations of well known properties of gratings. In particular, an equivalence rule concerning the far-field properties (diffraction efficiencies) of shallow and deep gratings is valid for the near-field zone above the grooves (the exception to this rule exhibits only the EFD inside the grooves, where for deep gratings one or more flow curls can be found).

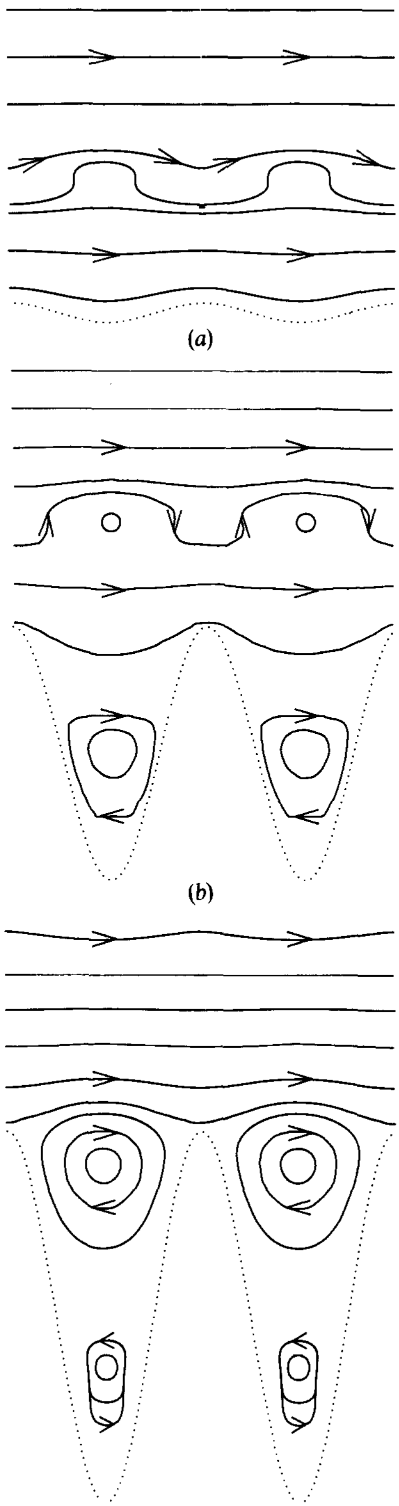



Figure 6. Energy flow distribution above the surface of the grating described in figure 5. In (a) $h/d = 0{\cdot}10$; in (b) $h/d = 1{\cdot}30$; in (c) $h/d = 1{\cdot}93$.

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