IEICE TRANS. ELECTRON., VOL.E90–C, NO.2 FEBRUARY 2007

PAPER Special Section on Recent Progress in Electromagnetic Theory and Its Application

# Scattering of TE Plane Wave from Periodic Grating with Single Defect

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**SUMMARY** This paper deals with the scattering of TE plane wave from a periodic grating with single defect, of which position is known. The surface is perfectly conductive and made up with a periodic array of rectangular grooves and a defect where a groove is not formed. By use of the modal expansion method, the field inside grooves is expressed as a sum of guided modes with unknown amplitudes. The mode amplitudes are regarded as a sum of the base component and the perturbed component due to the defect, where the base component is the solution in case of the perfectly periodic grating. An equation for the base component is obtained in the first step. By use of the base component, a new equation for the perturbed component is derived in the second step. A new representation of the optical theorem, relating the total scattering cross section with the reduction of the scattering amplitude is obtained. Also, a single scattering approximation is proposed to express the scattered field. By use of truncation, we numerically obtain the base component and the perturbed component, in terms of which the total scattering cross section and the differential scattering cross section are calculated and illustrated in figures.

***key words:*** *scattering, periodic grating, defect, TE plane wave, rectangular grooves, single scattering approximation*

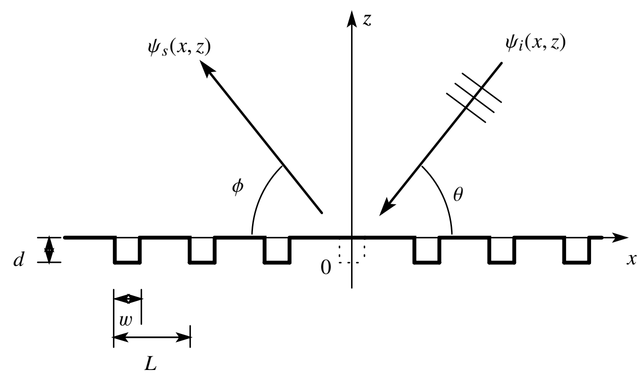


**Fig. 1** Scattering of TE plane wave from a periodic grating with single defect. The surface is a periodic array of rectangular grooves and has a defect where a groove is not formed. $\psi_i(x,z)$ is the incident wave and $\psi_s(x,z)$ is the scattered wave. $\theta$ is the angle of incidence, $\phi$ is the scattering angle, $L$ is the period of surface, $w$ and $d$ are the width and the depth of groove.

## 1. Introduction

In electronics, many devices such as memory chips and LCD electrodes have periodic structure with rectangular parallel lines. Defects in such periodic structure have been a serious problem for years. As a simple model of the periodic structure with defect, this paper studies the wave scattering from a periodic array of grooves with single defect shown in Fig. 1. This problem is practically important for developping an optical method of measurement and inspection.

There are many works [1]–[7] on the scattering and diffraction by a single groove, a finite number of grooves and a periodic array of grooves without any defects. However, there has not been studied the scattering from a periodic grating with defects.

This paper deals with the scattering of TE plane wave from a one-dimensional periodic grating with single defect, of which position is known. The surface is perfectly conductive and made up with a periodic array of rectangular grooves and a defect where a groove is not formed. By use of the modal expansion method [8], the field inside the grooves is expressed as a sum of guided modes with unknown mode amplitudes. The mode amplitudes are regarded as a sum of the base components and the perturbed components due to the defect, where the base component is the solution in case of the perfectly periodic grating without any defect. An equation for the base component is obtained in the first step. By use of the base component, a new equation for the perturbed component is derived in the second step.

We obtain a new representation of the optical theorem, which relates the total scattering cross section with the reduction of the scattering amplitude. To evaluate the scattering property approximately, we introduce a single scattering approximation, which is written only by the base component of the guided modes.

By use of truncation, we numerically obtain the base component and the perturbed component, in terms of which the total scattering cross section and the differential scattering cross section are calculated and illustrated in figures.

## 2. Mathematical Formulation of the Problem

### 2.1 Periodic Grating with Single Defect

Let us consider a periodic array of rectangular grooves with a single defect at $x = 0$ (See Fig. 1). We write such an array as

$$z = f(x) = -d\left[\sum_{n=-\infty}^{\infty} u(x-nL|w) - u(x|w)\right], \tag{1}$$

where $L$ is the period, $w$ and $d$ are the width and the depth of the groove. Here, $u(x|w)$ is a rectangular groove defined

Manuscript received May 17, 2006.
Manuscript revised September 3, 2006.

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DOI: 10.1093/ietele/e90–c.2.312

as

$$u(x|w) = \begin{cases} 1, & |x| \le w/2, \\ 0, & |x| > w/2. \end{cases} \tag{2}$$

It has the orthogonal property such that

$$u(x - mL|w)u(x - nL|w) = \delta_{mn}u(x - mL|w), \quad (m, n = 0, \pm 1, \pm 2, \cdots), \tag{3}$$

where $\delta_{mn}$ is Kronecker's delta. The Fourier transform of $u(x|w)$ is calculated as

$$U(q) = \int_{-\infty}^{\infty} u(x|w)e^{-iqx}dx = 2\frac{\sin(qw/2)}{qw}w, \tag{4}$$

which will be used later to obtain the scattered field.

For convenience, we put $k_L$ and $k_w$ as

$$k_w = \frac{\pi}{w}, \ \ k_L = \frac{2\pi}{L}, \tag{5}$$

and we define an auxiliary function $s_l(q)$ as follows.

$$s_l(q) = \int_{-\infty}^{\infty} u(x|w)\sin(lk_w(x + w/2))e^{-iqx}dx \tag{6}$$

$$= \frac{1}{2i}\Big[U(q-lk_w)e^{il\pi/2} - U(q+lk_w)e^{-il\pi/2}\Big], \tag{7}$$

where $l$ is integer. Figure 2 illustrates $s_l(q)$ for $l = 1, 4, 7$ with width the $w = 1.3\lambda$, where $\lambda$ is wavelength. $s_l(q)$ becomes a real even function for odd integer $l$, and an imaginary odd function for even integer $l$. Note that $s_l(q) \sim 1/q^2$ when $|q|$ becomes large. This auxiliary function $s_l(q)$ takes the phase shift by $e^{-iqmL}$ with the shift of $x$ by $mL$.

$$\int_{-\infty}^{\infty} u(x-mL|w)\sin(lk_w(x+w/2-mL))e^{-iqx}dx = e^{-iqmL}s_l(q). \tag{8}$$

We denote the $y$ component of the electric field by $\Psi(x, z)$, which satisfies the Helmholtz equation

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2\right]\Psi(x, z) = 0, \tag{9}$$

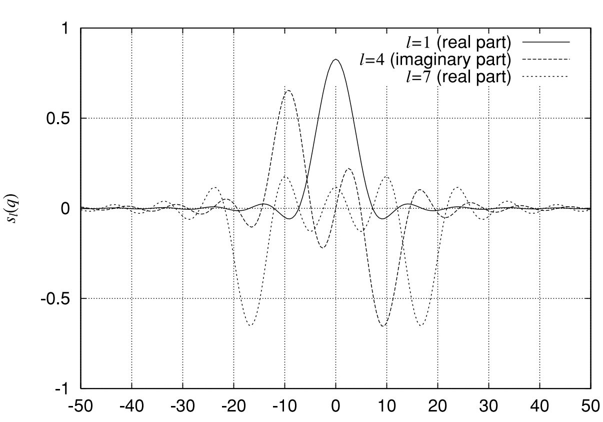


**Fig. 2** Auxiliary function $s_l(q)$ against wave number $q$ for $l = 1, 4, 7$ with width $w = 1.3\lambda$, $\lambda$ is wavelength.

in the region $z > f(x)$. Here, $k = 2\pi/\lambda$ is wavenumber. We consider that the surface is perfectly conductive. On the surface $z = f(x)$, the wave field $\Psi(x, z)$ satisfies the Dirichlet condition,

$$\Psi(x, z)|_{z=f(x)} = 0. \tag{10}$$

We write the incident plane wave $\psi_i(x, z)$ as

$$\psi_i(x, z) = e^{ipx}e^{-i\beta_0(p)z}, \ \ p = -k\cos\theta, \tag{11}$$

$$\beta_m(p) = \beta_0(p+mk_L) = \sqrt{k^2-(p+k_Lm)^2}, \tag{12}$$

$$Im[\beta_m(p)] \ge 0, \ \ (m = 0, \pm 1, \pm 2, \cdots), \tag{13}$$

where $\theta$ is the angle of incidence (See Fig. 1) and $Im$ stands for imaginary part.

## 2.2 Diffraction from a Perfectly Periodic Grating

First, we consider a perfectly periodic case without defect. We write such a perfectly periodic surface $f_p(x)$ as

$$z = f_p(x) = -d\sum_{n=-\infty}^{\infty} u(x-nL|w). \tag{14}$$

For the region $z \ge 0$, we put the $y$ component of the electric field $\hat{\Psi}_1(x, z)$ as a sum of the incident wave $\psi_i(x, z)$ and the diffracted wave $\psi_d(x, z)$ due to the periodicity of the surface,

$$\hat{\Psi}_1(x, z) = e^{ipx}e^{-i\beta_0(p)z} + \psi_d(x, z), \tag{15}$$

$$\psi_d(x, z) = e^{ipx}\sum_{m=-\infty}^{\infty} A_m e^{imk_Lx+i\beta_m(p)z}. \tag{16}$$

Here, $A_m$ is the amplitude of the $m$th order diffracted wave. On the other hand, by use of the modal expansion method [8], we write the $y$ component of the electric field inside the grooves $\hat{\Psi}_2(x, z)$ as a sum of the guided modes,

$$\hat{\Psi}_2(x, z) = \sum_{n=-\infty}^{\infty} u(x - nL|w)e^{ipnL}\left[\sum_{l=1}^{\infty} Q_l^s \times \sin(lk_w(x+w/2-nL))\frac{\sin(\gamma_l(z+d))}{\gamma_l}\right], \tag{17}$$

$$\gamma_l = \sqrt{k^2 - \left(\frac{\pi l}{w}\right)^2}, \tag{18}$$

where $Q_l^s$ is the amplitude of the guided mode which we call the base component, and $\gamma_l$ is the propagation constant of the $l$th guided mode. Note that the number of the guided modes starts from $l = 1$ since there is no constant mode for TE case.

Let us obtain the energy conservation relation for the perfectly periodic case. Using the identity $Im[\mathrm{div}\hat{\Psi}_1\mathrm{grad}\hat{\Psi}_1^*] = 0$ and the fact that $\hat{\Psi}_1\mathrm{grad}\hat{\Psi}_1^*$ is a periodic function with the period $L$, we obtain after some manipulation,

$$Im\left[\int_{-L/2}^{L/2}\hat{\Psi}_1(x, z)\frac{\partial}{\partial z}\hat{\Psi}_1^*(x, z)dx\right] = 0, \tag{19}$$

where $z > 0$. Substituting (15) and (16) into (19), we get

$$\beta_0(p) = \sum_{m=-\infty}^{\infty} Re[\beta_m(p)]|A_m|^2, \tag{20}$$

which is the well known energy conservation relation. Here, $Re$ stands for the real part and $Re[\beta_m(p)]|A_m|^2$ is the $m$th order diffraction power, which will be illustrated below.

### 2.3 Solution for a Perfectly Periodic Grating

Let us determine $A_m$ and $Q_l^s$ from the continuity of both the electric field and the magnetic field at $z = 0$.

From $\hat{\Psi}_1(x, 0) = \hat{\Psi}_2(x, 0)$, we get

$$\begin{aligned} e^{ipx}\left[1+\sum_{m=-\infty}^{\infty} A_m e^{imk_L x}\right] &= \sum_{n=-\infty}^{\infty} u(x-nL|w)e^{ipnL} \times \left[\sum_{l=1}^{\infty} Q_l^s \right. \\ &\quad \left. \times \sin(lk_w(x+w/2-nL))\frac{\sin(\gamma_l d)}{\gamma_l}\right]. \end{aligned} \tag{21}$$

Multiplying $e^{-imk_L x}$ and integrating over one period $L$, we get

$$A_m = -\delta_{m0} + \frac{1}{L}\sum_{l=1}^{\infty} Q_l^s \frac{\sin(\gamma_l d)}{\gamma_l} s_l(p+mk_L). \tag{22}$$

Next, from $\sum_{n\neq 0} u(x-nL|w)[\partial\hat{\Psi}_1/\partial z - \partial\hat{\Psi}_2/\partial z]_{z=0} = 0$, we get

$$\begin{aligned} &\sum_{n=-\infty}^{\infty} u(x-nL|w)e^{ipx} \\ &\quad \times\left[-i\beta_0(p)+i\sum_{m=-\infty}^{\infty}\beta_m(p)A_m e^{imk_L x}\right] \\ &= \sum_{n=-\infty}^{\infty} u(x-nL|w)e^{ipnL}\sum_{l=1}^{\infty} Q_l^s \\ &\quad \times \sin(lk_w(x+w/2-nL))\cos(\gamma_l d). \end{aligned} \tag{23}$$

Taking Fourier transform after multiplying $u(x - mL|w) \times \sin(lk_w(x + w/2 - mL))$, we obtain

$$\begin{aligned} &i\sum_{m=-\infty}^{\infty} \beta_m(p)A_m s_l(-p-mk_L) \\ &\quad = i\beta_0(p)s_l(-p)+\frac{wQ_l^s}{2}\cos(\gamma_l d). \end{aligned} \tag{24}$$

From (22) and (24), $A_m$ and $Q_l^s$ can be determined. Note that for the normal incidence $\theta = 90°$ $(p = 0)$, $Q_l^s$ vanishes for even numbers $l = 2, 4, 6, \cdots$ since $s_l(0)$ in the right hand side of (24) becomes 0 for even $l$ and $\beta_m(0)A_m s_l(-mk_L)$ and $\beta_{-m}(0)A_{-m}s_l(mk_L)$ cancel each other. This will be discussed later.

In the following section, we will obtain the scattered wave by using $\hat{\Psi}_1(x, z)$ and $\hat{\Psi}_2(x, z)$.

### 2.4 Scattering from a Periodic Grating with Single Defect

A single defect in a periodic grating generates the scattering. We express such scattering as a perturbation from the diffracted wave for the perfectly periodic case. Thus, we write for $z > 0$,

$$\Psi_1(x, z) = \hat{\Psi}_1(x, z) + \psi_s(x, z), \tag{25}$$

$$\psi_s(x, z) = e^{ipx}\int_{-\infty}^{\infty} a(s)e^{isx+i\beta_0(p+s)z}ds, \tag{26}$$

where $\psi_s(x, z)$ is the scattered wave due to the defect and $a(s)$ is the amplitude of the scattered wave. Since $\psi_s(x, z)$ is scattered from the single defect, $\psi_s(x, z)$ satisfies the radiation condition, that is, $\psi_s \sim e^{ikr}/\sqrt{r}$ $(r = \sqrt{x^2 + z^2})$ and decays at $r \to \infty$. This property will be used below.

On the other hand, we write the wave field inside the grooves $\Psi_2(x, z)$ as a sum of the wave field for the perfectly periodic grating and the fluctuated term $\psi_g(x, z)$ due to the defect.

$$\begin{aligned} \Psi_2(x, z) &= \hat{\Psi}_2(x, z) + \psi_g(x, z), \\ \psi_g(x, z) &= \sum_{n=-\infty}^{\infty} u(x-nL|w)e^{ipnL} \\ &\quad \times \sum_{l=1}^{\infty} q_l^{(n)} \sin(lk_w(x+w/2-nL))\frac{\sin(\gamma_l(z+d))}{\gamma_l} \\ &\quad -u(x|w)\sum_{l=1}^{\infty} Q_l^s \sin(lk_w(x+w/2))\frac{\sin(\gamma_l(z+d))}{\gamma_l}. \end{aligned} \tag{27}$$

Here, $q_l^{(n)}$ is the perturbed amplitude of the $l$th guided mode in the $n$th groove. Note that $q_l^{(0)} \equiv 0$ for all $l$ since a groove is not formed at $n = 0$.

### 2.5 Optical Theorem and Scattering Cross Section

Let us obtain the optical theorem for the single defect case. Since $\psi_s(x, z)$ decays proportional to $(x^2 + z^2)^{-1/4}$, $\hat{\Psi}_1 \mathrm{grad}\psi_s^*$, $\psi_s \mathrm{grad}\hat{\Psi}_1^*$ and $\psi_s \mathrm{grad}\psi_s^*$ vanish at $|x| \to \infty$. Further, $\hat{\Psi}_1 \mathrm{grad}\hat{\Psi}_1^*$ is a periodic function of $x$ with the period $L$. Using these facts and the identity $Im[\mathrm{div}(\hat{\Psi}_1 + \psi_s)\mathrm{grad}(\hat{\Psi}_1 + \psi_s)^*] = 0$, we obtain after some manipulation,

$$\begin{aligned} &\lim_{N\to\infty} Im\left[\int_{-(N+\frac{1}{2})L}^{(N+\frac{1}{2})L} \Psi_1(x, z)\frac{\partial}{\partial z}\Psi_1^*(x, z)dx\right] \\ &= \lim_{N\to\infty} Im\left[\int_{-(N+\frac{1}{2})L}^{(N+\frac{1}{2})L} \hat{\Psi}_1(x, z)\frac{\partial}{\partial z}\psi_s^*(x, z)\right. \\ &\quad \left. +\psi_s(x, z)\frac{\partial}{\partial z}\hat{\Psi}_1^*(x, z)+\psi_s(x, z)\frac{\partial}{\partial z}\psi_s^*(x, z)dx\right] = 0, \end{aligned} \tag{28}$$

where $z > 0$. Here, we have applied (19).

Substituting (15), (16) and (26) into (28), we get a new representation of the optical theorem, which is written as

$$P_c = \Phi_s, \tag{29}$$

$$P_c = -\frac{2}{k}\sum_{m=-\infty}^{\infty} Re[\beta_m^*(p)]Re[a(k_L m)A_m^*], \tag{30}$$

$$\Phi_s = \frac{1}{k}\int_{-\infty}^{\infty} Re[\beta_0(p+s)]|a(s)|^2 ds. \tag{31}$$

Here, $P_c$ is related to the reduction of the scattering amplitude and $\Phi_s$ expresses the total scattering cross section. The optical theorem (29) can be used to estimate accuracy of a numerical calculation. It is an extension of the forward scattering theorem [9], [10]. The total scattering cross section can be rewritten as

$$\frac{1}{k}\int_{-\infty}^{\infty} Re[\beta_0(p+s)]|a(s)|^2 ds = \frac{L}{2\pi}\int_0^{\pi}\sigma(\phi|\theta)d\phi, \tag{32}$$

where $\phi$ is the scattering angle and $\sigma(\phi|\theta)$ is the differential scattering cross section per period,

$$\sigma(\phi|\theta) = \frac{2\pi k\sin^2\phi\,|a(-k\cos\phi - p)|^2}{L}, \tag{33}$$

which has no dimension.

### 2.6 Scattered Wave Field and Single Scattering Approximation

In this section, we determine $a(s)$ and $q_l^{(n)}$ to solve the single defect case. From the continuity of both the electric field and the magnetic field, the equations to obtain $a(s)$ and $q_l^{(n)}$ are derived.

Since $\Psi_1(x,0) = \Psi_2(x,0)$ means $\psi_s(x,0) = \psi_g(x,0)$, we get

$$\begin{aligned} e^{ipx}\int_{-\infty}^{\infty} a(s)e^{isx}ds &= \sum_{n=-\infty}^{\infty} u(x-nL|w)e^{ipnL} \\ &\times\sum_{l=1}^{\infty} q_l^{(n)}\sin(lk_w(x+w/2-nL))\frac{\sin(\gamma_l d)}{\gamma_l} \\ &-u(x|w)\sum_{l=1}^{\infty} Q_l^s\sin(lk_w(x+w/2))\frac{\sin(\gamma_l d)}{\gamma_l}. \end{aligned} \tag{34}$$

Taking Fourier transform after multiplying $e^{-i(p+s')x}/2\pi$, we obtain the amplitude of the scattered wave $a(s)$ as

$$a(s) = \frac{1}{2\pi}\sum_{l=1}^{\infty} s_l(p+s)\frac{\sin(\gamma_l d)}{\gamma_l} \times\left[\sum_{n=-\infty}^{\infty} e^{-isnL}q_l^{(n)} - Q_l^s\right]. \tag{35}$$

When the depth $d$ is not so large that the resonance does not occur in the grooves of the grating, the term related to the first order guided mode $l = 1$ may become large. However, when the resonance occurs in the grooves, that is, the value of the depth $d$ satisfies $\sin(\gamma_1 d) = 0$, the summation on $l$ starts from $l = 2$, so the property of the scattering may become different. In such a case, the term related to the second order guided mode $l = 2$ may give large effect in the scattering. This will be discussed later.

On the other hand, from $\sum_{n\neq 0} u(x-nL|w)[\partial\Psi_1/\partial z - \partial\Psi_2/\partial z]_{z=0} = 0$, we obtain $\sum_{n\neq 0} u(x-nL|w)[\partial\psi_s/\partial z - \partial\psi_g/\partial z]_{z=0} = 0$. Then, we get

$$\begin{aligned} &\sum_{n=-\infty}^{\infty} u(x-nL|w)e^{ipx}\int_{-\infty}^{\infty} i\beta_0(p+s)a(s)e^{isx}ds \\ &\quad -u(x|w)e^{ipx}\int_{-\infty}^{\infty} i\beta_0(p+s)a(s)e^{isx}ds \\ &= \sum_{n=-\infty}^{\infty} u(x-nL|w)e^{ipnL}\sum_{l=1}^{\infty} q_l^{(n)} \\ &\quad \times\sin(lk_w(x+w/2-nL))\cos(\gamma_l d). \end{aligned} \tag{36}$$

Taking Fourier transform after multiplying $u(x-mL|w) \times\sin(lk_w(x+w/2-mL))$, we obtain

$$i\,(1-\delta_{m0})\int_{-\infty}^{\infty}\beta_0(p+s)s_l(-p-s)e^{ismL}a(s)ds = \frac{w}{2}\cos(\gamma_l d)q_l^{(m)}. \tag{37}$$

Substituting (35) into (37), we get the equation for the perturbed component $q_l^{(n)}$ as

$$\sum_{j=1}^{\infty}\sum_{n=-\infty}^{\infty} C_{lm}(j,n)q_j^{(n)} = \sum_{j=1}^{\infty} Q_j^s\left[C_{lm}(j,0) + \delta_{m0}\delta_{lj}\frac{w}{2}\cos(\gamma_l d)\right]. \tag{38}$$

Here, $Q_j^s$ is the base component obtained from (22) and (24), and $C_{lm}(j,n)$ is given as

$$\begin{aligned} C_{lm}(j,n) &= (1-\delta_{m0})\frac{i}{2\pi}\frac{\sin(\gamma_j d)}{\gamma_j}e^{-ip(m-n)L} \\ &\times\int_{-\infty}^{\infty}\beta_0(s')s_l(-s')s_j(s')e^{is'(m-n)L}ds' \\ &-\delta_{mn}\delta_{lj}\frac{w}{2}\cos(\gamma_l d), \end{aligned} \tag{39}$$

where the integral can be easily evaluated numerically because the integrand decays proportional to $1/s'^3$ when $|s'| \to \infty$. Here, $C_{lm}(j,n)$ represents coupling between the $j$th guided mode at the $n$th groove and the $l$th guided mode at the $m$th groove. Note that $C_{lm}(j,n)$ is independent of $p$. We will calculate $C_{lm}(j,n)$ numerically to solve (38) for the perturbed component $q_l^{(n)}$, in terms of which $a(s)$ is calculated.

On the other hand, if $q_l^{(n)}$ is small, the approximated amplitude of the scattered wave $\hat{a}(s)$ could be calculated from (35) only with $Q_l^s$ as

$$\hat{a}(s) = -\frac{1}{2\pi}\sum_{l=1}^{\infty} s_l(p+s)\frac{\sin(\gamma_l d)}{\gamma_l}Q_l^s, \tag{40}$$

which we call the single scattering approximation. $\hat{a}(s)$ is written only by the base component $Q_l^s$ neglecting $q_l^{(n)}$, which is the effect of coupling between neighboring grooves. We will compare this single scattering approximation $\hat{a}(s)$ with numerical solution $a(s)$ in what follows.

## 3. Numerical Examples

Let us obtain some numerical examples for $L = 2\lambda$.

Since (38) is a linear equation for infinitely many unknown $q_l^{(n)}$, it is still an open question how to solve (38). However, we attempt to solve this by use of truncation. We introduce the truncation number $N_d$ of the diffraction orders, the truncation number $N_m$ of the guided modes inside the groove and the number of the grooves $N_g$. This means that we assume

$$\begin{aligned} A_m &= 0, \quad |m| > N_d, \\ Q_l^s &= 0, \quad l > N_m, \\ q_l^{(n)} &= 0, \quad |n| > N_g, \;\; l > N_m, \end{aligned} \tag{41}$$

in the summation (22) and (24) and we take into account the perturbed effect in the grooves between $n = -N_g$ and $N_g$, In this paper, we set

$$N_d = 7, \;\; N_m = 15, \quad N_g = 7. \tag{42}$$

Thus, $[A_m]$ becomes a $(2N_d + 1)$ vector, $[Q_l^s]$ becomes an $N_m$ vector and $[q_l^{(n)}]$ becomes an $(N_m) \times (2N_g + 1)$ matrix in the calculation below. We numerically calculate the base component $Q_l^s$ and $C_{lm}(j, n)$ to solve (38) for the perturbed component $q_l^{(n)}$. Then, we obtain a numerical solution $a(s)$ to calculate the optical theorem and the scattering cross section.

First, we consider the perfectly periodic case. Figure 3 illustrates the relative diffraction power against the angle of incidence $\theta$ for the depths $d = 0.1\lambda$ (upper figure) and $d = 0.542\lambda$ (lower figure) with the width $w = 1.3\lambda$. The power of incident wave is normalized to 1. The line '(0)' means the relative power of the 0th order Floquet mode, i.e., $Re[\beta_0(p)]|A_0|^2/\beta_0(p)$, and the line '(1)' that of the 1st order Floquet mode, and so on. The energy error is always less than $10^{-14}$ in these cases. It suggests that the truncation numbers $N_d$ and $N_m$ are sufficient for the perfectly periodic case. For $d = 0.1\lambda$, the power of the 0th mode is quite large. However, for $d = 0.542\lambda$, which satisfies $\sin(\gamma_1 d) = 0$, the powers of the $-2$nd mode and the $-3$rd mode become large and that of the 0th mode decreases when the angle of incidence is between 30° and 70°.

For the case with single defect, we calculate the optical theorem by truncating the number of the grooves with $N_g$. Figure 4 illustrates the total scattering cross section $\Phi_s$ and the reduction of the scattering amplitude $P_c$ against the angle of incidence $\theta$ for the widths $w = 0.7\lambda$, $1.0\lambda$, $1.3\lambda$ with the depths $d = 0.1\lambda$ (upper figure) and $0.542\lambda$ (lower fig-

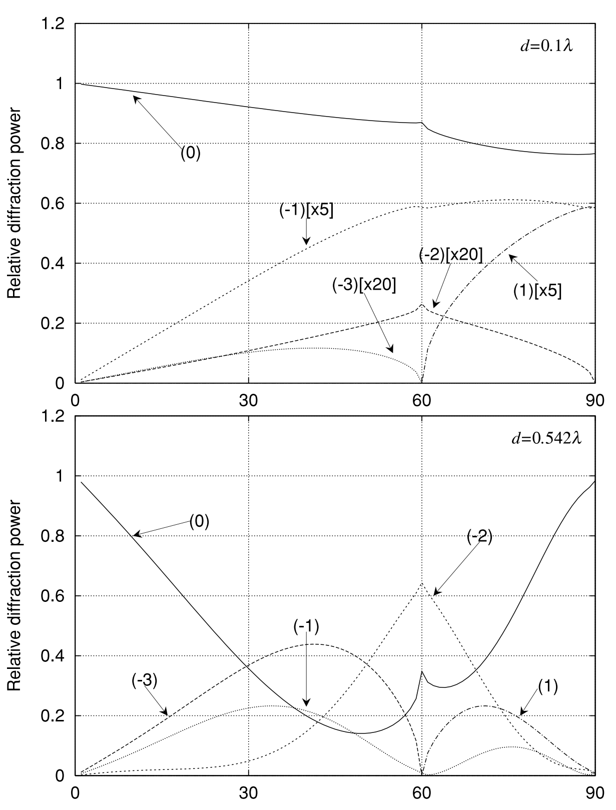


**Fig. 3** Relative diffraction power against the angle of incidence $\theta$ for depths $d = 0.1\lambda$ (upper figure), $0.542\lambda$ (lower figure) with period $L = 2\lambda$ and width $w = 1.3\lambda$, $\lambda$ is wavelength. Power of incident wave is normalized to 1. In the upper figure for $d = 0.1\lambda$, '[x5]' means that values are multiplied by 5 and '[x20]' means that values are multiplied by 20.

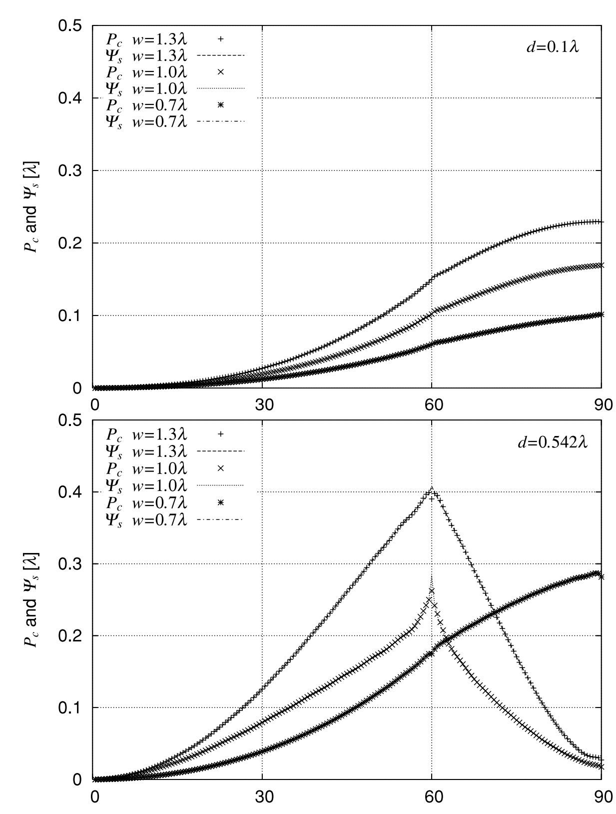


**Fig. 4** Optical theorem against the angle of incidence $\theta$ for widths $w = 0.7\lambda$, $1.0\lambda$, $1.3\lambda$ with period $L = 2\lambda$, depth $d = 0.1\lambda$ (upper figure) and $d = 0.542\lambda$ (lower figure), $\lambda$ is wavelength. Total scattering cross section $\Phi_s$ is drawn with line, while the reduction of scattering amplitude $P_c$ is shown with dots.

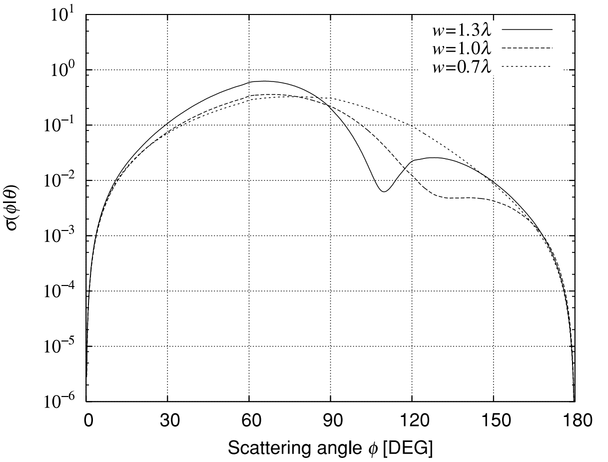


**Fig. 5** Differential scattering cross section $\sigma(\phi|\theta)$ for widths $w = 0.7\lambda$, $1.0\lambda$, $1.3\lambda$ with period $L = 2\lambda$, and depth $d = 0.1\lambda$, angle of incidence $\theta = 60°$, $\lambda$ is wavelength.

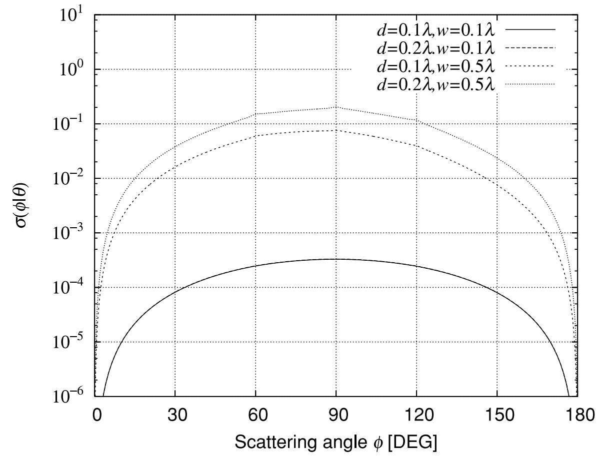


**Fig. 6** Differential scattering cross section $\sigma(\phi|\theta)$ when the widths of the groove are relatively small ($w = 0.1\lambda$ and $0.5\lambda$) with period $L = 2\lambda$, angle of incidence $\theta = 60°$ and depths $d = 0.1\lambda$ and $0.2\lambda$, $\lambda$ is wavelength.

ure). The total scattering cross section is drawn with lines, while the reduction of scattering amplitude is shown with dots. In both figures, the total scattering cross section $\Phi_s$ almost agrees with the reduction of the scattering amplitude $P_c$ in three cases of $w$. However, there are some cases in which relative error $Err^{opt} = |(\Psi_s - P_c)/P_c|$ becomes large. For $d = 0.1\lambda$, $Err^{opt}$ is less than 0.01, but, it becomes approximately 0.02 when $\theta$ is close to 60° where the 1st mode appears and the −3th mode disappears. For $d = 0.542\lambda$, $Err^{opt}$ is less than 0.02, but, it becomes approximately 0.1 when $\theta$ is close to 60°, and becomes approximately 0.2 when $\theta$ is close to 90° where the 2nd mode appears and the −2nd mode disappears. When $\theta < 20°$, $Err^{opt}$ increases up to 0.1 for both cases of $d$. These facts suggest that the truncation in (38) gives a reasonable solution in general, but is not good enough for several cases. Thus, practical methods of approximation must be studied to solve (38).

Figure 5 illustrates the differential scattering cross section $\sigma(\phi|\theta)$ for the widths $w = 0.7\lambda$, $1.0\lambda$, $1.3\lambda$ with the depth $d = 0.1\lambda$ and the angle of incidence $\theta = 60°$. The differential scattering cross section is determined by $s_l(q)$ in (35), which is the spectrum of the groove with the width $w$. Figure 6 illustrates $\sigma(\phi|\theta)$ when the widths of the groove are relatively small ($w = 0.1\lambda$ and $w = 0.5\lambda$) with the angle of incidence $\theta = 60°$. Calculations are done for two cases of the depths $d = 0.1\lambda$ and $0.2\lambda$. For $w = 0.1\lambda$, which is much smaller than the half wavelength, all order guided modes inside the grooves become cutoff. This makes little difference in the differential scattering cross section for different values of the depth $d$. Figure 7 illustrates $\sigma(\phi|\theta)$ for the angles of incidence $\theta = 90°$, 60°, 30° with the width $w = 1.3\lambda$ and the depths $d = 0.1\lambda$ (upper figure) and $0.542\lambda$ (lower figure). It is found that for $d = 0.1\lambda$, scattering is relatively strong in the direction of specular reflection. However, for $d = 0.542\lambda$, the differential scattering cross section seems symmetric with respect to $\phi = 90°$. It may be due to the fact that the resonance inside the grooves depends on the

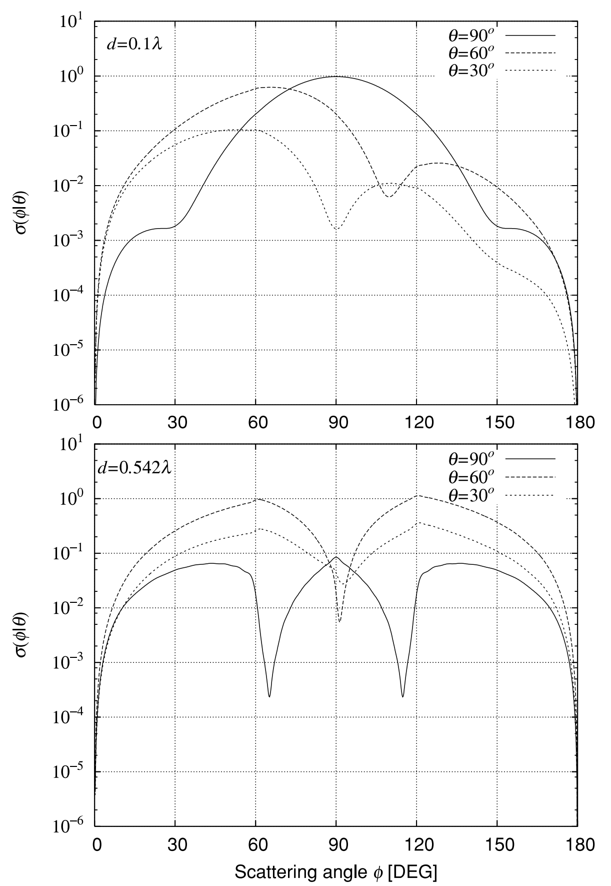


**Fig. 7** Differential scattering cross section $\sigma(\phi|\theta)$ for angles of incidence $\theta = 90°$, 60°, 30° with period $L = 2\lambda$, width $w = 1.3\lambda$, depth $d = 0.1\lambda$ (upper figure) and $0.542\lambda$ (lower figure), $\lambda$ is wavelength.

depth $d$ and the width $w$, but is independent of the angle of incidence $\theta$. In these cases, the term related to the second order guided mode (mainly $s_2(p+s)$) in (35) becomes large. For $\theta = 90°$, the scattering amplitude becomes small due to the fact that $Q_2^s$ vanishes for the normal incidence and the

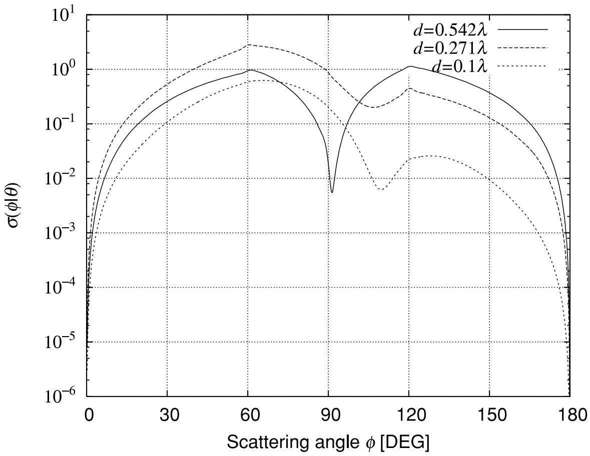


**Fig. 8** Differential scattering cross section $\sigma(\phi|\theta)$ for depths $d = 0.1\lambda$, $0.271\lambda$, $0.542\lambda$ with period $L = 2\lambda$, and width $w = 1.3\lambda$ and angle of incidence $\theta = 60°$, $\lambda$ is wavelength.

term related to the third order guided mode determines the scattering property. Figure 8 illustrates $\sigma(\phi|\theta)$ for the depths $d = 0.1\lambda$, $0.271\lambda$, $0.542\lambda$ with $w = 1.3\lambda$ and $\theta = 60°$. For $d = 0.1\lambda$ and $0.271\lambda$, the differential scattering cross section increases as the depth $d$ becomes large and the forward scattering around the direction of the specular reflection is relatively strong. However, for $d = 0.542\lambda$, the differential scattering cross section is smaller than that for $d = 0.271\lambda$ around the direction of specular reflection.

Figure 9 examines the single scattering approximation (40). Comparison of the numerical solution with the single scattering approximation is illustrated for the depths $d = 0.1\lambda$ (upper figure) and $0.542\lambda$ (lower figure) with the width $w = 1.3\lambda$ and $\theta = 60°$. For $d = 0.1\lambda$, the single scattering approximation (40) almost agrees with the numerical solution, which takes $q_l^{(n)}$ into account. However, for $d = 0.542\lambda$, the agreement becomes worse since some ripples appear in the scattering cross section due to the effect of the perturbed component $q_l^{(n)}$. It may suggest that when the depth of the grooves is not large the interaction between neighboring grooves may be small for TE incidence.

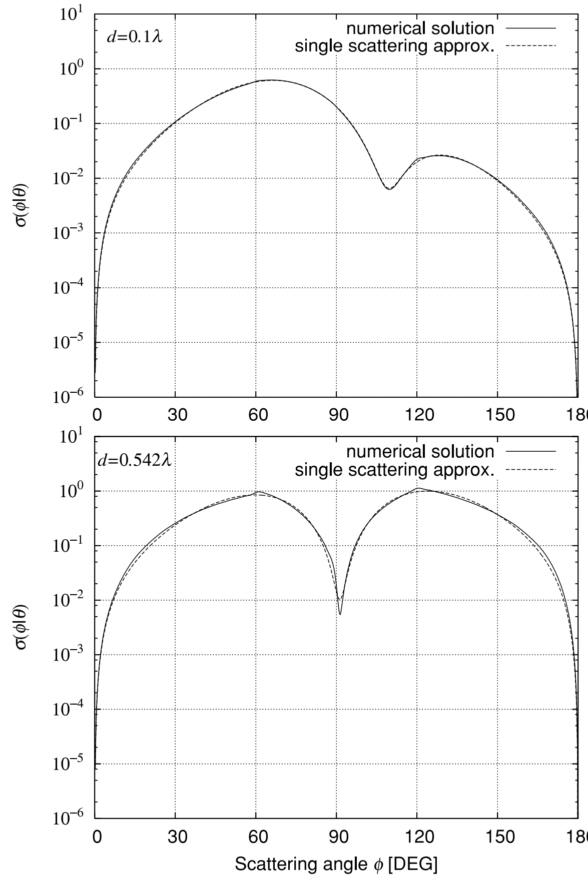


**Fig. 9** Comparison of numerical solution with the single scattering approximation for depths $d = 0.1\lambda$ (upper figure) and $0.542\lambda$ (lower figure), for period $L = 2\lambda$, width $w = 1.3\lambda$ and angle of incidence $\theta = 60°$, $\lambda$ is wavelength. The approximation is shown in dotted lines.

## 4. Conclusions

We considered a one-dimensional periodic grating with single defect, of which position is known. We took TE plane wave as an incidence, wrote the wave field above the grooves as a perturbation from the diffracted wave for the perfectly periodic case. We derived two sets of equations to determine the wave field from the boundary condition, and we obtained a new representation of the optical theorem, which relates the total scattering cross section with the reduction of the scattering amplitude. Further, we proposed the single scattering approximation given only by the base components for the perfectly periodic grating.

We found that the differential scattering cross section is determined by the spectrum of the groove. This property may be applicable to the measurement of the condition of surfaces combining with the other polarization. We found that when the guided mode in the grooves becomes resonant, the differential scattering cross section becomes almost symmetric even for oblique incidence. We found the single scattering approximation is useful when the depth of the groove is small.

In this paper, we obtained the scattered wave by use of truncation, and there are several cases in which relative error with respect to the optical theorem becomes large. It means that our truncation method is not good enough and practical methods of approximation must be studied to obtain a highly accurate solution.

Our discussion was limited to the case of TE incidence. It can be extended to TM case [11]. In this paper, we considered the single defect case in the periodic grating. However, there are other mathematical models of periodic grating with defects: one is a case with double or finite number of defects which positions are known. Another is a case with random defects, that is, the defect probability is known but their positions are unknown. It is theoretically interesting to consider such periodic gratings with defects. However, those cases will be left for the future studies.

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