Difference scattering field properties between periodic defect particles and three-dimensional slightly rough optical surface*

Cheng-Xian Ge(葛城显)[1], Zhen-Sen Wu(吴振森)[1,†], Jing Bai(白靖)[1], and Lei Gong(巩蕾)[2]

[1] School of Physics and Optoelectronic Engineering, Xidian University, Xi'an 710071, China
[2] School of Photoelectric Engineering, Xi'an Technological University, Xi'an 710021, China

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Based on the practical situation of nondestructive examination, the calculation model of the composite scattering is established by using a three-dimensional half-space finite difference time domain, and the Monte Carlo method is used to solve the problem of the optical surface with roughness in the proposed scheme. Moreover, the defect particles are observed as periodic particles for a more complex situation. In order to obtain the scattering contribution of defects inside the optical surface, a difference radar cross section is added into the model to analyze the selected calculations on the effects of numbers, separation distances, different depths and different materials of defects. The effects of different incident angles are also discussed. The numerical results are analyzed in detail to demonstrate the best position to find the defects in the optical surface by detecting in steps of a fixed degree for the incident angle.

Keywords: light scattering, difference scattering field, periodic particles, rough optical surface

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1. Introduction

The quality of the optical surface plays a crucial role in determining the properties of the optical system. The requirements of industry mean people must provide more effective methods to test the quality of the optical surface.[1–5] In the field of nondestructive examination, the optical surface is invariably observed as a surface without roughness. Research on rough surface[6,7] and the scattering properties of the half-space problem with multiple defect particles for an optical surface without roughness[8] has been discussed. It is well known that the roughness of the optical surface inevitably limits properties of the system.[9] So in order to find the defects of the optical surface timely and ensure the safety and reliability of the optical system, the optical surface must be observed as being slightly rough. Study on the scattering properties of the slightly rough optical surface with the targets is in accordance with the actual accident situation.

In the past several years, analyzing the scattering field to accurately determine the size, the shape and the material of a target has been demonstrated to be feasible, although it is complicated. A number of theoretical methods such as discrete dipole approximation[10–12] and discrete sources[13–15] method have been developed. Johnson used the method of the combination of standard grid and discrete dipole to investigate the composite electromagnetic scattering properties between two-dimensional (2D) rough surface and three-dimensional (3D) objects above/below the rough surface.[16] El-Shenawee used the steepest descent fast multipole method to investigate the electromagnetic scattering properties of the 2D layered rough surface with/without targets.[17] Hu and Chew used the non-uniform fast plane wave method to investigate the scattering properties between rough surface and 3D complex targets.[18] Fung et al. investigated the scattering properties of a rough surface by using a Gauss window function.[19] Moss *et al.*[20] used the three-wave method to study the electromagnetic scattering properties between a non-uniform rough surface and inside conductor. Li *et al.*[21] investigated the fast forward computation of a 3D perfect electric conductor (PEC) target in a 2D dielectric rough surface. A hybrid method based on the reciprocity theorem and the forward–backward method[22] has been used to solve the scattering of rough surface with a 2D target. The composite electromagnetic scattering by a ship-like target on the randomly rough sea surface also have been discussed by using the finite difference time domain (FDTD) method.[23–27] Although a lot of effort has been devoted to investigating the composite scattering between rough surface and target, there are very few composite scattering researches of the rough surface with more targets in laser wavelengths, especially in the case that there are periodic defect particles inside the optical surface. Light scattering is a powerful tool for controlling the optical surface quality. Investigation of light scattering by an optical surface through computer simulation is a reliable tool for investigating the properties and functional abilities of an optical system by defect particles with the optical surface.[28]

With the development of optical nondestructive examina-

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†Corresponding author. E-mail: wuzhs@mail.xidian.edu.cn

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tion, the size of the defect particle is generally observed to be on the order of micronmeter or submicronmeter.[29] So the scattering contribution of a slightly rough optical surface in the detection of the scattering intensity plays a crucial role, and the scattering contribution of defect particles is less. Only when the illumination width of incident wave is small, can the scattering contribution of the defect particles be valid.[30] In order to eliminate these uncertainties of the numerical results, the research on difference scattering field has been conducted. Johnson[31] first proposed the concept of the difference scattering field which calculates the scattering fields of a rough surface with and without the targets, and uses the difference between these two scattering fields to obtain the difference radar cross section (RCS). In this paper, we establish a half-space FDTD model into which the difference scattering field is added for analyzing the composite scattering properties. The primary purpose of this paper is to investigate the properties of the defect particles inside the optical surface and provide a theoretical basis for the nondestructive examination to find the defects reliably. The main schematic of the investigation in this paper is shown in Fig. 1.

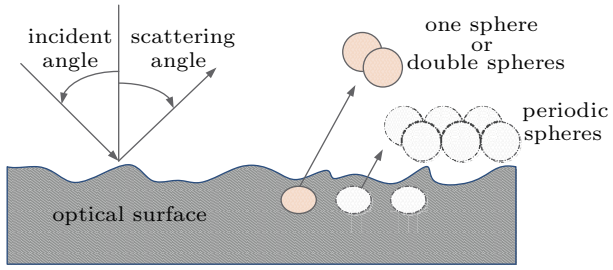


Fig. 1. (color online) Schematic of the spherical particles inside a slightly rough optical surface.

2. Establishment of calculation model

2.1. Theory of difference radar cross section in FDTD

In this paper, the half-space model of a slightly rough optical surface with the targets is of a 3D structure. According to the theory of 3D FDTD, the basic iterative equation of an electromagnetic field can be expressed as

$$E_x^{n+1}\left(i+\frac{1}{2},j,k\right), \tag{1}$$

$$E_y^{n+1}\left(i,j+\frac{1}{2},k\right), \tag{2}$$

$$E_z^{n+1}\left(i,j,k+\frac{1}{2}\right). \tag{3}$$

The above is the formula of an electric field in 3D FDTD. The formula of a magnetic field can also be obtained as follows:

$$H_x^{n+1/2}\left(i,j+\frac{1}{2},k+\frac{1}{2}\right), \tag{4}$$

$$H_y^{n+1/2}\left(i+\frac{1}{2},j,k+\frac{1}{2}\right), \tag{5}$$

$$H_z^{n+1/2}\left(i+\frac{1}{2},j+\frac{1}{2},k\right). \tag{6}$$

The meanings of the specific parameters in Eqs. (1)–(6) can be obtained from Ref. [19]. The theoretical basis of the FDTD method is not introduced in this paper.

In order to obtain the difference scattering field, the scattering by a slightly rough optical surface must be obtained by using the FDTD method with Eqs. (1)–(3) and (4)–(6) in the first place. This scattering field can be expressed as H_x', H_y', H_z' and E_x', E_y', E_z'. Next, the composite light scattering field between the slightly rough optical surface and defect particles can be calculated, which can be expressed as H_x'', H_y'', H_z'' and E_x'', E_y'', E_z''. Finally, the difference scattering fields H_x, H_y, H_z and E_x, E_y, E_z can be calculated as follows:

$$H_x = H_x'' - H_x',\ \ H_y = H_y'' - H_y',\ \ H_z = H_z'' - H_z', \tag{7}$$

$$E_x = E_x'' - E_x',\ \ E_y = E_y'' - E_y',\ \ E_z = E_z'' - E_z'. \tag{8}$$

From Eqs. (7)–(8), H_x, H_y, H_z and E_x, E_y, E_z can be used for near-far field extrapolation by reciprocity theorem. The difference RCS can be obtained to analyze the properties between defect particles and the slightly rough optical surface. Figure 2 summarizes the process of getting the difference scattering field:

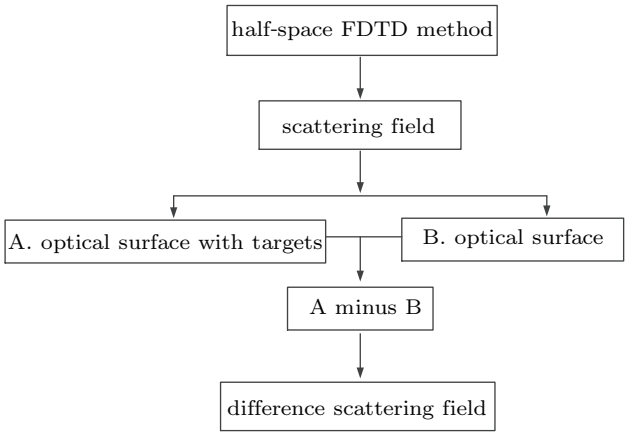


Fig. 2. Flow chart of getting the difference scattering field.

2.2. Model of slightly rough optical surface

In this paper, the slightly rough optical surface is simulated by the Monte Carlo method. Assuming that the proportion of the rough surface is S, in x and y directions, and the sample intervals are equal, the height of each (x,y) is[32]

$$z(x,y) = \frac{1}{L_x L_y}\sum_{m=-N/2}^{N/2-1}\sum_{n=-N/2}^{N/2-1} F(K_{xm},K_{yn})\,\mathrm{e}^{(\mathrm{j}K_{xm}x+\mathrm{j}K_{yn}y)}. \tag{9}$$

In the above formula

$$L_x \times L_y = S, \tag{10}$$

$$F(K_{xm},K_{yn})=2\pi\sqrt{L_xL_yW(K_{xm},K_{yn})}\times\begin{cases}[N(0,1)+\mathrm{j}N(0,1)]/\sqrt{2}m, & n\neq 0,N/2,\\ N(0,1)m \text{ or } n=0, & N/2,\end{cases} \tag{11}$$

where $N(0,1)$ is the Gauss random number, of which the mean valve is 0 and variance is 1, and

$$K_{xm}=2\pi n/L_x,\quad K_{yn}=2\pi n/L_y,$$

$$F(K_{xm},K_{yn})=F^*(-K_{xm},-K_{yn}),$$

$$F(K_{xm},-K_{yn})=F^*(-K_{xm},K_{yn}), \tag{12}$$

$$W(K_{xm},K_{yn})=\delta^2\frac{l_xl_y}{4\pi}e(-K_{xm}^2l_x^2/4-K_{yn}^2l_y^2/4), \tag{13}$$

where l_x and l_y are the correlation lengths, δ is the root mean square (RMS) height.

In this paper, the rough surface is of 3D structure. From Eq. (9), it can be concluded that it is four program loops in the program calculation, which inevitably wastes a lot of computing time. This problem can be solved by using the Fourier transform to calculate Eq. (9).

2.3. Model of half-space FDTD

In this paper established is the composite scattering model of the slightly rough optical surface with targets by using the half-space FDTD method, which is different from the usual FDTD method and the three-wave method.[20] The calculation model is shown in Fig. 3. The connective boundary and the output boundary have only one side. And the rough surface in the half-space FDTD model is directly connected to the absorbing boundary. The perfectly matched layer (PML) is used as the absorbing boundary. The volume of grids, which is above the rough surface, is divided into the scattering field region and the total field region. Between these two regions, the incident waves are generated, and a transformation is used to convert the scattering field into a far zone field for RCS and difference RCS. Although infinite space is simulated by the limited space in the FDTD method, possible errors near the edge of the side can influence the correctness of the numerical result. In order to eliminate this possible error, the windowing function is applied to the connective boundary.[19] Figure 3 shows the primary calculation model of defect particles inside the slightly rough optical surface in this paper.

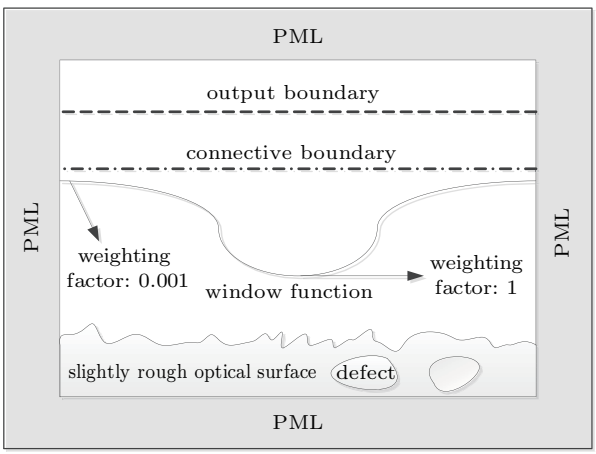


Fig. 3. Side view of 3D half-space FDTD model.

3. Results of numerical calculation

Figure 4 shows the 3D geometry of the electromagnetic scattering. $\boldsymbol{k}_\mathrm{i}$ and $\boldsymbol{k}_\mathrm{s}$ are the incident wave vector and the scattering wave vector, respectively. The incident angle and the incident azimuth angle can be expressed as θ and φ. The scattering angle and the scattering azimuth angle are respectively θ_s and φ_s. The polarizing angle is α. In this paper, the numerical results such as RCS and difference RCS are all normalized, which can be represented as a normalized radar cross section (NRCS).

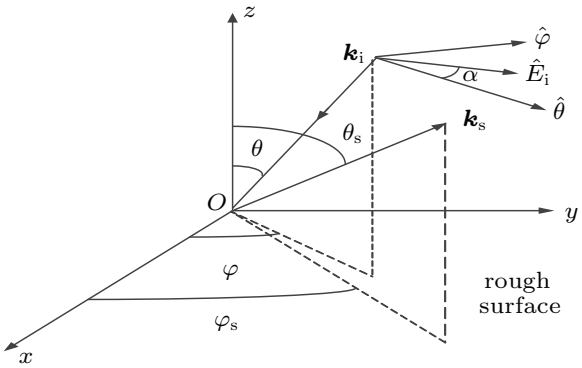


Fig. 4. Geometry for the scattering.

In order to prove the correctness of the calculation model which is established in this paper, the result of the calculation model is compared with the result which is obtained by using Kirchhoff approximation (KA).[33,34] For simulation, PEC is chosen as the rough surface. The size of the discrete grid in the FDTD method is $\lambda/10$ where λ is the incident wavelength whose value is 0.3 m. The correlation lengths l_x and l_y are both 1λ. The RMS height δ is 0.08λ. The incident angle is 20°. The size of the rough surface is $51.2\lambda\times 51.2\lambda$. The reason why these parameters are used to make a comparison is that they are in accordance with the condition of numerical dispersion stability of the FDTD method and the condition of KA. The calculation model of the half-space FDTD method can be shown in Fig. 3. KA is an approximation method of which the calculation model can be shown in Fig. 4. The final value of NRCS is an average value of 50 NRCS samples. It is because the height of the 3D rough surface is random, and the average value can eliminate the error of the numerical results. The result which makes a comparison is shown in Fig. 5. It indicates

that the calculation model is proved to be right. In Fig. 5, there is a small difference between two curves for the NRCS. It is because the NRCS sample size is not enough to completely eliminate the possible errors, and the KA method is imprecise at large scattering angles. In the next section, after a statement of the calculation model, various situations involving possibility knowledge are investigated.

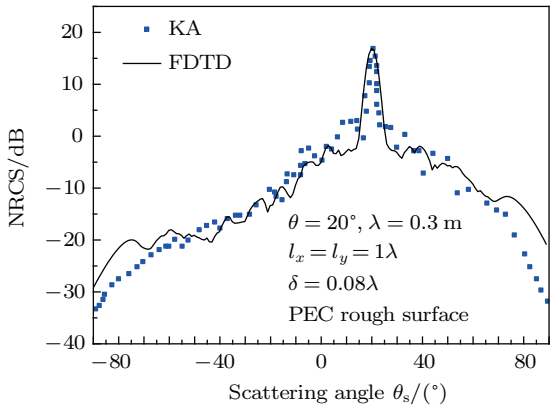


Fig. 5. (color online) Comparison of the plot of NRCS versus the scattering angle between the half-space FDTD and KA.

3.1. Double particles inside the slightly optical rough surface

Figure 6 shows the schematic of double defect particles inside the slightly rough optical surface. l is the separation distance between two particles. h is the depth of double particles. For simulation, the size of the rough surface is fixed. K9 glass is chosen as the slightly rough optical surface of which the refractive index is $(1.52, 0)$. The size of the optical surface is $35\lambda \times 35\lambda$. The incident angle is 20°. φ and α are both 0°. The incident wavelength λ is 0.6328 μm. The correlation lengths l_x and l_y are both 0.43 μm, and the RMS height δ of the slightly rough optical surface is 0.051 μm. A bubble is chosen as the defect particle. The refractive index of the bubble is $(1, 0)$. h is 2λ. l is $4\sqrt{2}\lambda$. The radius of the defect particle is 1λ. These parameters are in accordance with those under the actual condition of the optical surface with slight roughness for non-destructive examination. These parameters are used to investigate the selecting principle of parameters in the following.

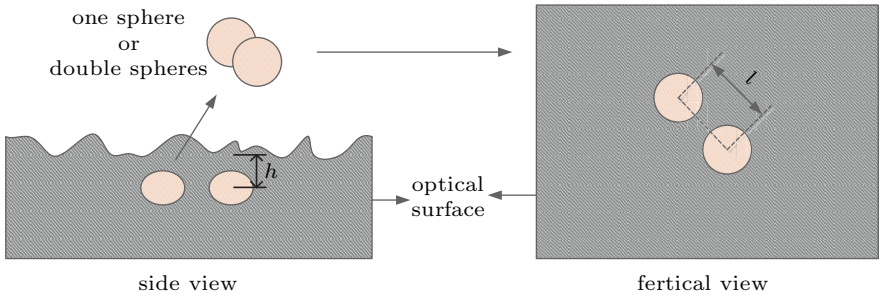


Fig. 6. (color online) Schematic diagram of slightly rough optical surface with double particles.

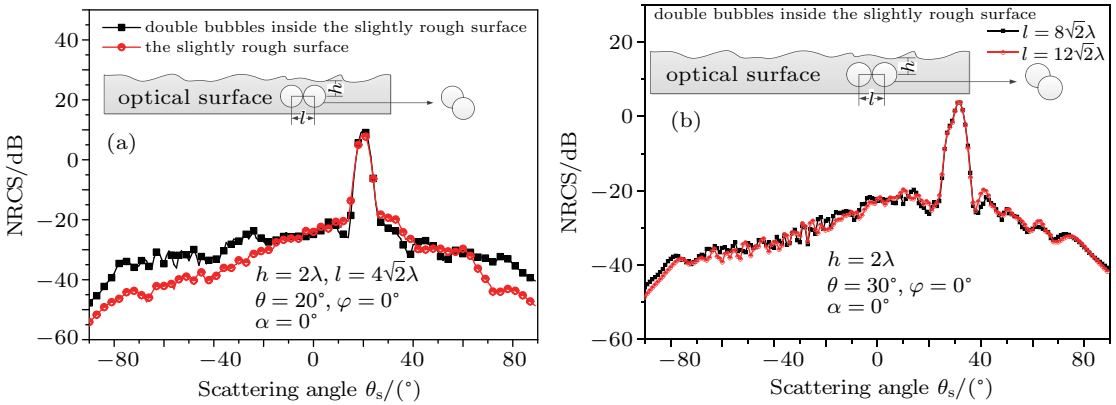


Fig. 7. (color online) Double defect particles inside the optical surface: (a) NRCSs of slightly rough optical surface with/without defects; (b) NRCSs of double defects with different separation distances.

Figure 7 shows the composite scattering properties of the slightly rough optical surface with double defect particles. In Fig. 7(a), the incident angle is 20°. It shows the difference between the optical surfaces with/without the defects. Due to the fact that the incident angle is small, when the scattering angle is 20°, the peak values of the curve appear, which mainly depend on the scattering contribution of the optical surface, and the scattering contribution of the defects is covered up. But the composite scattering field can increase at the large scattering angles. In Fig. 7(b), the incident angle is 30°. It shows that the scattering contribution of double defect particles for the composite scattering field is less. As the separation be-

tween two particles increases, there is no difference between two curves for composite scattering. It is because the slightly rough optical surface is much larger than the defects, and with the increase of l, the interaction between two particles disappears. Only when the illumination width of the incident wave is smaller or the particles are larger, can the scattering contribution of defect particles be valid. So the scattering properties of a more complex situation such as periodic particles inside the optical surface must be investigated.

3.2. Periodic particles inside the slightly rough optical surface

Figure 8 shows the schematic of the slightly rough optical surface with periodic defect particles. p is the separation between two particles for the periodic particles in the x direction. q is the separation in the y direction. Periodic $x(px)$ is the number of the particles in the x direction. Periodic $y(py)$ is the number of the particles in the y direction.

In order to investigate the properties of the periodic defect particles inside the slightly rough optical surface expediently, in Fig. 9, the periodic defect particles are observed as PEC and the bubble. The NRCS is calculated to study the composite scattering properties. The refractive index of the slightly rough optical surface (K9 glass) is $(1.52, 0)$. The incident angle θ is 20°. φ and α are 0°. The wavelength λ is 0.6328 μm which is equal to the radius of the particle. The correlation lengths l_x and l_y are both 0.43 μm, and the RMS height δ of the slightly rough optical surface is 0.051 μm. h is 2λ. The size of the optical surface is fixed to be $35\lambda \times 35\lambda$. px and py are both 16. p and q are both 2λ. For these parameters, it can be concluded that there are 16×16 periodic defect particles inside the slightly rough optical surface.

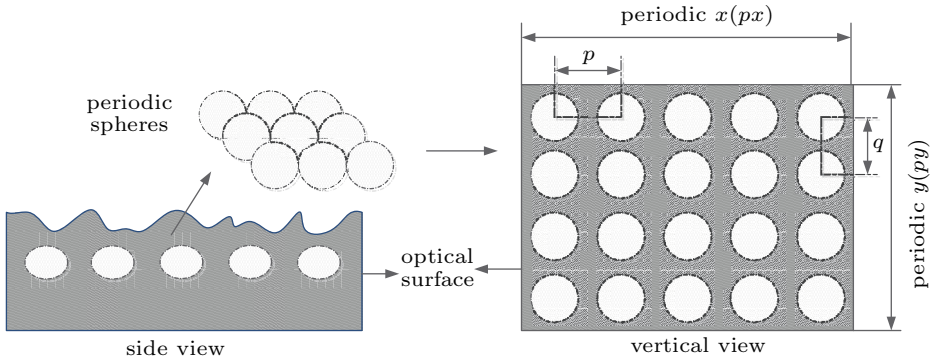


Fig. 8. Schematic diagram of slightly rough optical surface with periodic particles.

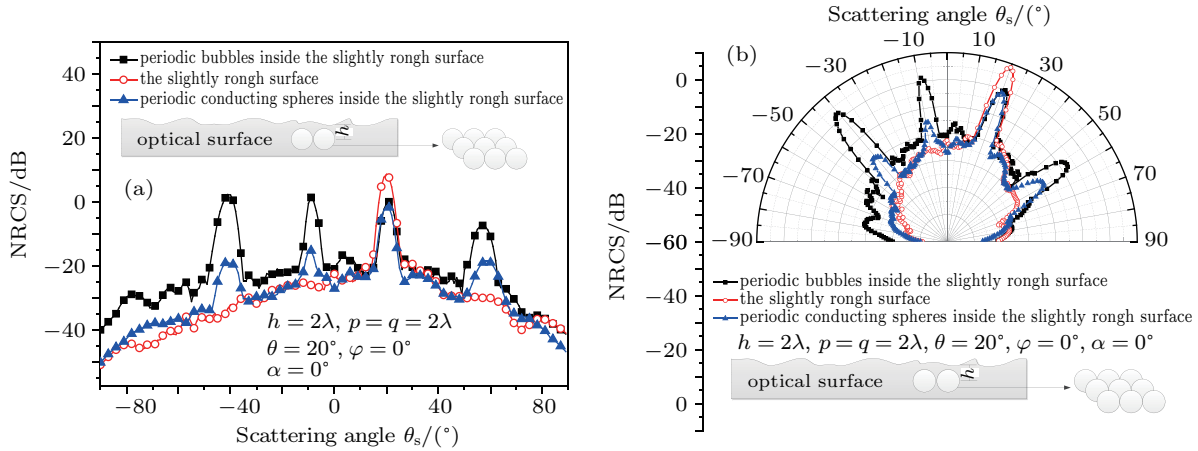


Fig. 9. (color online) Light scattering of the periodic defect particles inside the slightly rough optical surface: (a) x–y plot; (b) polar plot.

In Fig. 9, the solid triangle curve indicates that the particle is PEC; the empty circle curve indicates that it is the slightly rough optical surface without defects; the solid square curve indicates that periodic bubbles are inside the slightly rough optical surface. Figure 9(a) shows that the periodic bubbles are different from double particles inside the optical surface. The number of peaks of the curve for periodic defects is more than that of the curve for the slightly rough optical surface. For the periodic particles inside the optical surface, it can also be known that the values of curves are smaller at a scattering angle of 20° compared with the situation for optical surface without targets. It is because the scattering contribution of the periodic particles plays a crucial role in the composite scattering. So it is important to investigate the difference scattering field properties and calculate the difference RCS of the periodic defect particles, which can solely obtain the scattering

contribution of periodic particles.

Figure 9(b) shows that the interval between the peaks of curves for periodic particles is about 30°. This helps to detect the existence of the periodic defect particles inside the optical surface by measuring the NRCS in steps of 30° for a fixed incident angle. It is a remarkable fact that this is only for the case that the size of the optical surface is $35\lambda \times 35\lambda$. px and py are both 16.

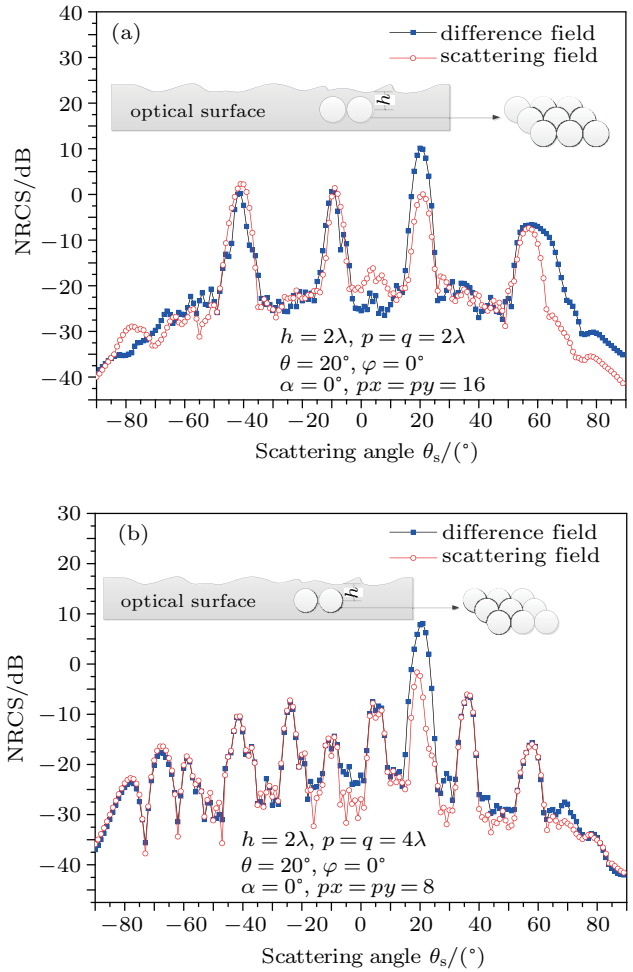


Fig. 10. (color online) Difference field and scattering field for the periodic defect particles inside the slightly rough optical surface: (a) $px = py = 16$; (b) $px = py = 8$.

Next, the main emphasis is placed on the investigation of the difference scattering field. The study of the difference scattering field of the periodic defect particles can help us investigate the composite scattering properties better to provide a more useful theoretical basis for nondestructive examination. In the following calculations, all parameters are the same as those used in Fig. 9. According to Fig. 8, it can be concluded that figure 10(a) shows 16×16 periodic particles inside the optical surface and figure 10(b) shows 8×8 periodic particles inside the optical surface.

Figure 10 indicates that the scattering contribution of periodic particles plays a crucial role in the composite scattering, and the difference scattering field is slightly smaller at the scattering angle of 20°. It is due to the fact that the optical surface is slightly rough, and the interaction between defect particles and optical surface is strongest.

In this paper, the incident angle can be arbitrary. The best incident angle to test the quality of the optical surface is very crucial. A comparison of Fig. 11(a) with Fig. 11(b) indicates that in the cases that the incident angles are 20°, 50°, and 70°, the positions of peaks for the curve invariably move with the increase of the incident angle . When the scattering angle is equal to the incident angle, one of the peaks appears necessarily, and the other peaks of the curve have a fixed interval in between for the fixed incident angle. Due to the fact that the calculation model is based on the half-space FDTD method and the connective boundary only has one side, it is not easy to explain the features of the curve at the large scattering angle. In order to avoid this problem and investigate the properties of the composite scattering field conveniently, the incident angle of 20° is chosen as the best incident angle in this paper.

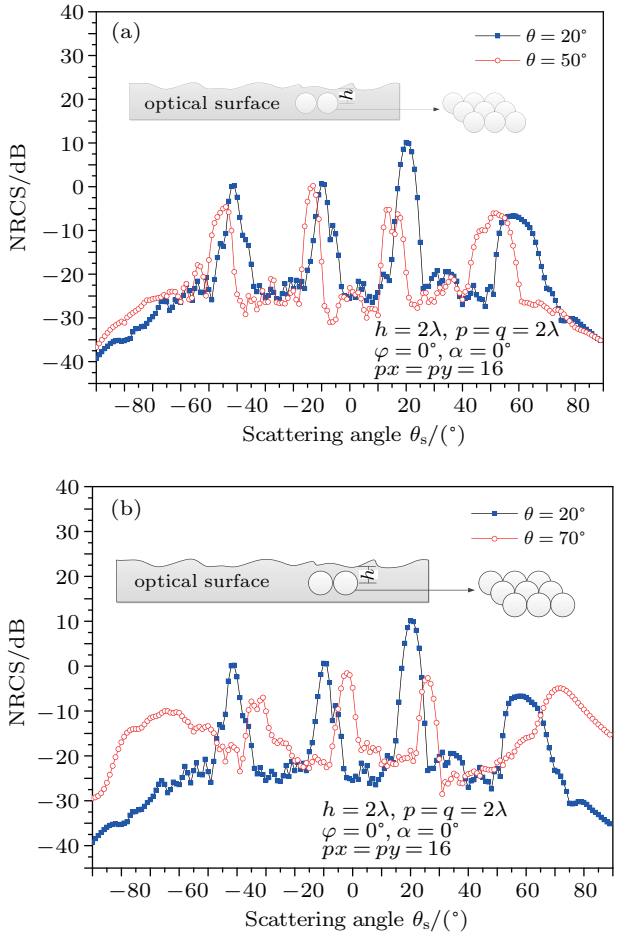


Fig. 11. (color online) Difference scattering fields for different incident angles: (a) $\theta = 20°, 50°$; (b) $\theta = 20°, 70°$.

As is well known, the defect particles with different positions and separations have different scattering properties. In Fig. 8, px and py can be arbitrary. In order to obtain the effects of px and py on the composite scattering, different values of px and py are used to investigate the scattering properties. In Fig. 12, the solid triangle curve indicates that the values of

px and py are both 8, $p = q = 4\lambda$; empty circle curve indicates that $px = py = 16$, $p = q = 2\lambda$; solid curve indicates that $px = py = 11$, $p = q = 3\lambda$. From Fig. 8, it can be concluded that as the px changes, p will change at the same time, py and q have the same variation rule. It is because the size of the slightly rough optical surface is fixed. Figure 12 shows that with the increase of the value of px and py, the number of the peaks of the curve will decrease. The interval between two peaks will increase and be about fixed. It indicates that in the field of nondestructive examination, with the values of p and q increasing, the difference scattering field of the periodic defect particles will be more sensitive.

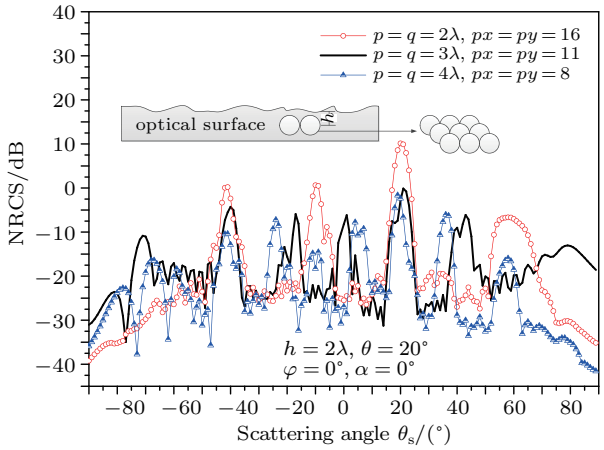


Fig. 12. (color online) Difference scattering fields for different values of periodic x and periodic y.

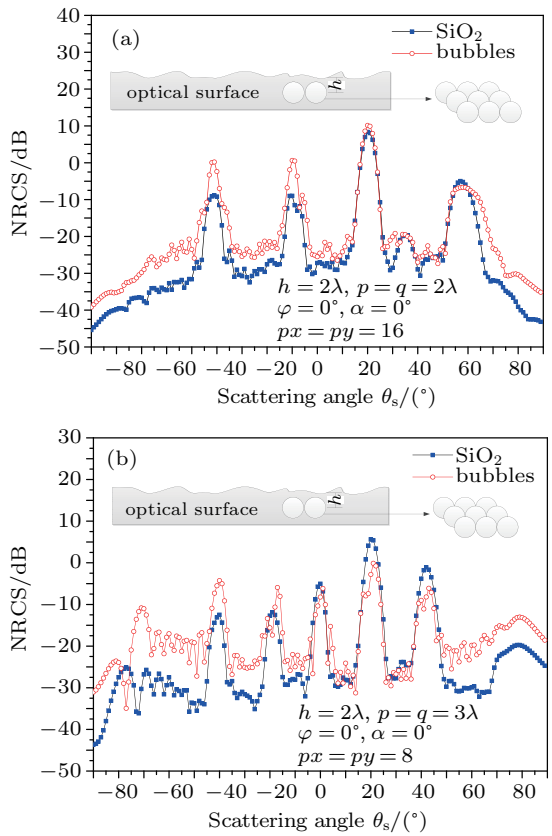


Fig. 13. (color online) Difference scattering fields for different materials with (a) $px = py = 16$; (b) $px = py = 8$.

Figure 13 shows different materials of the periodic defect particles inside the optical surface. The refractive index of the SiO_2 is $(1.67, 0)$. It can be concluded that the difference RCS of the SiO_2 is less than that of the bubbles inside the optical surface. But in the direction where the scattering angle is larger than 20°, the peaks of the curve exhibit the abnormal changes. It is due to the presence of coherent scattering. This result indicates that in order to find the materials of the periodic defect particles reliably, the detecting position should be in the mirror direction for an incident angle.

Figure 14 is the schematic of different depths for periodic defect particles. Figure 15 shows the effects of the depth of the periodic defect particles on the composite scattering. The periodic defect particles are bubbles. It can be indicated that the difference scattering field will decrease with depth increasing. The difference between the curves at the scattering angle of 60° is larger. So the depth of the periodic defect particles inside the optical surface can be measured mainly at the position where the peaks of the curve appear.

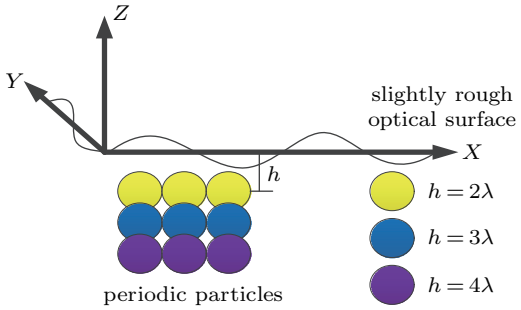


Fig. 14. (color online) Schematic of different depths for periodic defect particles inside the optical surface.

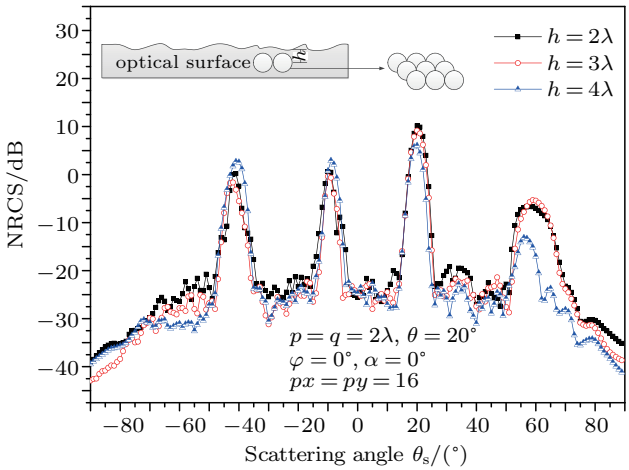


Fig. 15. (color online) Difference scattering fields for different depths of the periodic defect particles.

4. Conclusions and perspectives

In this work, the half-space FDTD model is established to investigate the properties between a slightly rough optical surface and defect particles. The accuracy of the calculation model is verified by comparing with that given by KA. This

model is better than the other methods because it has a wide range of applications. In order to investigate the properties of the defects better, the theory of difference scattering field and roughness is added into the calculation model of half-space FDTD to mainly discuss the periodic defect particles inside the slightly rough optical surface. The effects of various cases on the results are investigated in detail, which provide a theoretical basis for the nondestructive examination to find the defects quickly and reliably. The results indicate that first, the difference scattering field can be used to analyze the scattering properties better, second, for detecting the periodic defect particles, the incident angle of 20° is chosen as the best incident angle and the NRCS can be measured with an interval of fixed degree for the incident angle, third, with the increase of the separation distance, the difference scattering field of the periodic defect particles will be more sensitive. Finally, in order to find the material of periodic defect particles, the detecting position can be the mirror direction for the incident angle. The results in this paper can also provide a theoretical basis for optical film, as well as for the optical performance design of nanometer structure. More investigations are still required before reaching the final goal. Improving the algorithm and considering more cases of the composite scattering will be desired in our future work.

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