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Comparative analysis of two methods for calculating reflectance of black silicon

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Abstract. **We report a detailed numerical simulation of the reflection of visible light from a sub-wavelength grating with a rectangular profile on the silicon surface. Simulation is carried out by the effective refractive index method and rigorous coupled-wave analysis. The dependences of the reflectance on the grating depth, fill factor and angle of incidence for TE and TM polarisations are obtained and analysed. Good agreement between the results obtained by the two methods for grating periods of ~100 nm is found. The possibility of reducing the polarised light reflectance to about 1 % by adjusting the depth and the grating fill factor is demonstrated. The characteristics of the Brewster effect manifestation (pseudo-Brewster angle) in the system under study are considered. The possibility of the pseudo-Brewster angle existence and its absence for both polarisations of the incident light is shown as a function of the parameters of a rectangular nanostructure on the surface.**

Keywords: *black silicon, sub-wavelength grating, reflectance, pseudo-Brewster angle.*

1. Introduction

Black silicon is a promising material for modern optoelectronics. The study of numerous publications on black silicon has revealed the absence of a single definition of the concept, which is not surprising given the relative newness of the term that was first introduced in 1995 [1]. In this paper, we use a generalised definition [2], which, in our opinion, most fully complies with modern trends and interests of researchers in this field: black silicon is a nanostructured silicon surface that can reduce the reflectance in the optical range.

Interest in this material, which has a small, up to 1%, reflectance in the visible range, is associated with the development of a new family of efficient photovoltaic power sources [3]. Of great interest is its ability to generate terahertz radiation [4]. In our opinion, black silicon is also a very promising material for the rapidly developing field of research related to the creation of perfect absorbers of optical radiation [5]. One can but mention in this connection a recent high-profile paper [6], whose authors found bactericidal properties of this material.

The high absorption coefficient of black silicon is due to its surface relief, which represents a spatial nanograting with a characteristic period, significantly smaller than the wavelength of absorbed optical radiation. In practice, the specific parameters of the relief are determined by the technological possibilities and applied purposes. To date, most of the published studies on the optical properties of black silicon refer to the case of a chaotic needle structure in which a single element of the nanostructure is a vertically oriented nanorod. These structures are primarily interesting for applications in photovoltaic [3].

Recent years have been characterised by a rapid development of technologies, which make it possible to produce gratings with a controlled profile and a period of 50–100 nm, including comb-shaped structures, on the silicon surface. Such structures may, in our opinion, be of interest from the point of view of the further development of optoelectronic element base, i.e., the fabrication of polarisation-sensitive optical radiation absorbers.

In connection with the experiments on the interaction of optical radiation with such nanostructures, there is a need in the evaluation of their optical properties and, consequently, in the construction of appropriate calculation methods. Note that if the study of the interaction of broadband optical radiation with black silicon is important for applications in the field of photovoltaic, it is no less important and promising in the investigation of the interaction at a fixed wavelength, primarily for the development and improvement of modern micro- and nano-optoelectronic devices as well as nondestructive methods of technological control and characterisation of nanomaterials. In this regard, very useful are the effects related to the behaviour of the pseudo-Brewster angle as a function of the nanostructure parameters [7]. However, when it comes to black silicon, this effect is not sufficiently studied.

Generally, it should be noted that interest in black silicon has been initially associated with the ability to precisely control the etching of silicon in real time [1]. However, to date, the reflection properties of black silicon based on comb nanostructures with a rectangular profile as functions of the geometric parameters of the structure, depth, fill factors and polarisation in the range of characteristic periods of 50–100 nm, to our knowledge, has not been studied in detail.

The above circumstance determines the main objective of this paper. Thus, if the geometry of the periodic structure is known, its reflective properties can be accurately calculated using the rigorous coupled-wave analysis (RCWA) method. This method gives the exact solution of the problem of scat-

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tering by a periodic structure of arbitrary profile. However, its use in a particular spectral range requires careful analysis of the convergence of the solutions, especially for the TM polarisation of light. At the same time, important (particularly for optimisation problems) is the development of approximate methods of calculation of the optical properties of black silicon and metamaterials.

Using the method of effective refractive index (ERI), one can obtain analytical expressions that allow the properties of the experimental nanometamaterials to be predicted and optimised. The use of the ERI method is possible when the smallness of the relief period, as compared with the wavelength of the optical radiation, allows the averaging of the permittivity in the structure under consideration. The exact RCWA method and the approximate ERI method can be complementary; however, it is first needed to compare and analyse the results of the calculation by both methods in the range of interest (periods of 50–100 nm) for different depths and fill factors of the structures. We also consider this problem in this paper, because, as far as we know, the results of such studies in the range of nanostructure parameters in question on silicon surfaces have not been published, despite the great interest in the subject matter as a whole [8, 9]. We have chosen a structure on a silicon surface with a rectangular profile and a period of 70 nm, to which the basic dependences presented in the Figures of this paper correspond, although in our study we have also analysed the dependences for the periods of 50–150 nm.

2. Calculation by the effective refractive index method

As already noted, this method is not accurate, because it is based on averaging the refractive index in the grating region. Depending on the particular problem, different approaches to the calculation of the average refractive index are possible [10].

Consider the geometry of our problem in the right-handed coordinate system xyz. The surface of the silicon substrate lies in the xy plane. A grating with a rectangular profile, which occupies the region $0 < z < d$ over the depth, is formed on the substrate surface. The grating vector is directed along the x axis, and the grating profile does not depend on the coordinate y. It is assumed that a plane polarised optical wave is incident on the grating surface. The plane of incidence coincides with the xz plane, and the angle of incidence is equal to θ. In this geometry, this wave can be represented as a superposition of two TE- and TM-polarised waves [11], which are then treated independently. In this case, a classical definition is used for such polarisations [12]: for a transverse electric wave (TE polarisation), the electric vector is perpendicular to the plane of incidence, while for a transverse magnetic wave (TM polarisation), the electric vector is parallel to the plane of incidence.

The silicon substrate has a refractive index n_s, and the medium bordering the substrate has a refractive index n_0, which hereafter will be equal to unity. The fill factor f is defined as the ratio of the width of the grating line to its period T. If one can average the refractive index in the region of the grating, then this region of the grating can be replaced by a thin film with a corresponding effective refractive index. In this case, the problem of finding the reflectance of incident optical radiation having a wavelength λ_0 is reduced to the well-known problem of reflection from a layered medium [12]. The correctness of averaging is supported by the smallness of the spatial scale on which the refractive index $\sim T/2 \sim$ 30 nm changes, as compared with the wavelength of optical radiation in the visible range (about 500 nm). However, this is not sufficient to replace the grating by a medium with some ERI; therefore, below the thus obtained results will be compared with the results of rigorous calculations.

To calculate ERI, we will replace for simplicity the rectangular grating by a set of plates, infinitely extended in the z and y directions. This allows one to use the arguments [12] and easily obtain a solution for ERI in such a system in two cases:

1. The electric field strength vector of the optical wave lies in the plane yz, i.e., in the plane of the plates.

We believe that the electric field inside each plate and in the gap between the plates can characterise electric field strengths E_1 and E_2, respectively. We also assume that the field strengths are related with electric induction through the conventional expressions $D_2 = \varepsilon_2 E_2$ and $D_1 = \varepsilon_1 E_1$, where ε_2 and ε_1 are the permittivities associated with refractive indices: $\varepsilon_2 = n_2^2, \varepsilon_1 = n_1^2$. Proceeding from the obvious boundary condition $E_1 = E_2$, we have

$$D_1/\varepsilon_1 = D_2/\varepsilon_2. \quad (1)$$

Next, determining the average permittivity as

$$\tilde{\varepsilon} = \tilde{D}/\tilde{E}, \quad (2)$$

where $\tilde{D} = D_1(1-f) + D_2 f$ and $\tilde{E} = E_1(1-f) + E_2 f$, we obtain

$$\tilde{\varepsilon} = \frac{D_1(1-f) + D_2 f}{E_1(1-f) + E_2 f}, \quad (3)$$

which in view of (1) gives the expression for the average permittivity in the case of TE polarisation

$$\tilde{\varepsilon} = \varepsilon_1(1-f) + \varepsilon_2 f. \quad (4)$$

In view of the previously introduced notations, we obtain for ERI at this polarisation

$$\tilde{n}_{||} = \left[n_0^2(1-f) + n_s^2 f\right]^{1/2}. \quad (5)$$

2. The electric field strength vector of the incident wave is directed along the x axis, i.e., perpendicular to the plane of the plates.

This case is similar to the previous one with the boundary condition $D_1 = D_2$. Then, we have

$$\varepsilon_1 E_1 = \varepsilon_2 E_2, \quad (6)$$

$$\tilde{\varepsilon} = \frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 f + \varepsilon_2(1-f)}, \quad (7)$$

$$\tilde{n}_{\perp} = \left[\frac{n_0^2 n_s^2}{n_0^2 f + n_s^2(1-f)}\right]^{1/2}. \quad (8)$$

Now we can replace the grating of depth d by a film of the same thickness, but with an effective refractive index $\tilde{n}$. As a result, we obtain a system, which represents a thin film with a known refractive index $\tilde{n}$ (medium 2), bordering medium 1 and bulk silicon (medium 3) on one side and on the other side, respectively. It is obvious that for a normally incident TE-polarised wave we have $\tilde{n} = \tilde{n}_{||}$, and for a TM-polarised wave we have $\tilde{n} = \tilde{n}_{\perp}$. The reflectance R with respect to intensity is given by the expression [12]

$$R = |r|^2 = \left| \frac{r_{12} + r_{23}\exp(2j\beta)}{1 + r_{12}r_{23}\exp(2j\beta)} \right|^2, \qquad (9)$$

where r_{12} and r_{23} are the Fresnel reflectances at the interface between the media $\beta = 2\pi\tilde{n}d\cos\varphi/\lambda_0$; and φ is the angle of refraction in the film (medium 2). In the calculations we assume that $n_0 = 1$, $n_s = 3.844 - 0.015j$ and $\lambda_0 = 650$ nm.

Figure 1 shows the thus obtained dependence of the reflectance R on the grating depth d at a fixed value of the fill factor $f = 0.5$ and $\theta = \varphi = 0$. As can be seen from these dependences, the reflectance for the TE and TM waves varies sinusoidally from 0.35, which corresponds to the unperturbed silicon surface, to 0.12. In this case, the period of the reflectance variation for TE and TM polarisations is ~100 and ~200 nm, respectively.

This change in the reflectance is quite significant, but it is known from the literature [13] that the reflectance of black silicon can be reduced to a few percent. Perhaps, this can be achieved by optimising the parameter f. We tested this hypothesis by changing the parameter f at a fixed value of the grating depth $d = 100$ nm. The corresponding dependences of the reflectance for the two polarisations are presented in Fig. 2 and confirm our assumption.

One can see that for TE polarisation the reflectance reaches a minimum ~0.02 at $f \sim 0.17$, and for TM polarisation the same minimum is achieved at $f \sim 0.72$. The most interesting feature of these curves is that they are clearly asymmetric, depending on f. At the same time, in first approximation the dependences for TE and TM polarisations can be considered mutually mirror-symmetric.

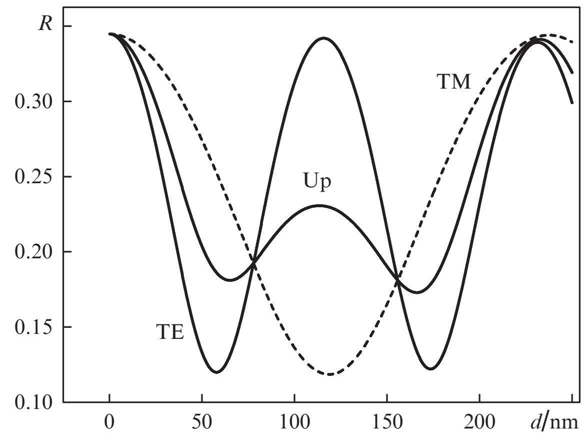

Figure 1. Dependences of the reflectance R on the grating depth d for TE and TM polarisations and unpolarised light Up at $f = 0.5$ and $\theta = 0$. Calculation by the ERI method.

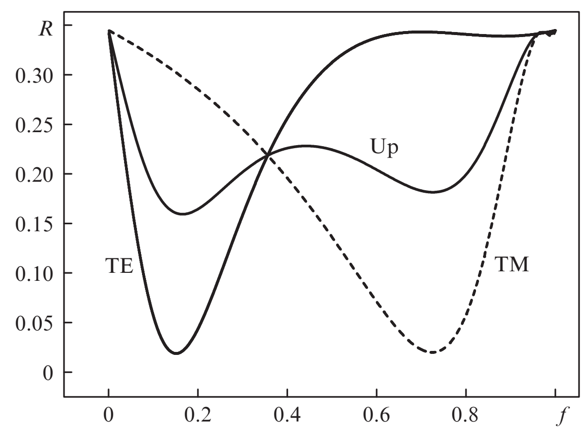

Figure 2. Dependences of the reflectance R on the fill factor f for TE and TM polarisations and unpolarised light Up at $d = 100$ nm and $\theta = 0$. Calculation by the ERI method.

3. Calculation by the RCWA method

A detailed description of the RCWA method can be found in the original paper [11] and in paper [14] devoted to its application. Therefore, here we confine ourselves to a brief description of the general principles of the method by the example of TE polarisation. The geometry of the problem is described in the previous section. Solutions in media 1 and 3 with allowance for the Floquet theorem are sought for in the form of propagating plane and evanescent waves:

$$E_y^{(1)}(x,z) = E_0\exp[-jk_0n_1(x\sin\theta + z\cos\theta)] + \sum_{i=-\infty}^{\infty} P_i\exp[-j(k_{xi}x - k_{zi}^{(1)}z)], \qquad (10)$$

$$E_y^{(3)}(x,z) = \sum_{i=-\infty}^{\infty} T_i\exp\{-j[k_{xi}x + k_{zi}^{(3)}(z-d)]\}, \qquad (11)$$

where P_i and T_i are the electric field amplitudes corresponding to the ith wave in media 1 and 3; $k_{xi} = k_0(n_1\sin\theta - i\lambda_0/\Lambda)$; $k_{zi}^{(1)} = (n_1^2k_0^2 - k_{xi}^2)^{1/2}$; and $k_{zi}^{(3)} = (n_3^2k_0^2 - k_{xi}^2)^{1/2}$.

In the region of the grating (medium 2) the electric and magnetic field strengths are written as an expansion in Fourier harmonics with the amplitudes that depend on the coordinate z:

$$E_y^{(2)}(x,z) = \sum_{i=-\infty}^{\infty} S_{yi}(z)\exp[-jk_{xi}x], \qquad (12)$$

$$H_x^{(2)}(x,z) = -j(\varepsilon_0/\mu_0)^{1/2} \sum_{i=-\infty}^{\infty} U_{xi}(z)\exp[-jk_{xi}x]. \qquad (13)$$

From these expressions we can obtain a system of matrix differential equations, which is solved by finding the eigenvectors and eigenvalues. Finally, the desired amplitude P_i and T_i of the fields and the associated reflectances are found by matching the fields on the boundaries of regions and solving the corresponding system of ordinary algebraic equations. In this case, the key parameter on which the accuracy and calculation time depend is the number of harmonics used in the expansion of the fields over the Fourier harmonics. Usually, in the case of metallic gratings with periods of ~1 μm at a wavelength of ~1 μm, the convergence for TE polarisation is achieved at ~10 harmonics. For TM polarisation the situation is much more complicated, and even at more than 100 harmonics the convergence is not guaranteed and each case requires a separate verification [15].

In our case, the convergence with an error of less than 0.5% is achieved when the total number of harmonics is $N > 10$ and $N > 140$ for TE and TM polarisations, respectively. The dependences of the reflectance on the grating depth and the fill factor are presented in Figs 3 and 4. Similarly to the previous case, the dependence on d can be characterised as sinusoidal, for TE polarisation the period being twice less than for TM polarisation. As for the dependence on the parameter f, it also retains the main characteristics obtained by the approximate method and mentioned above.

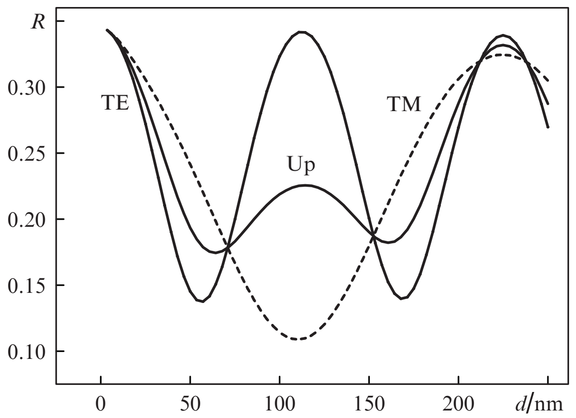

Figure 3. Dependences of the reflectance R on the grating depth d for TE and TM polarisations and unpolarised light Up at $f = 0.5$, $\theta = 0$ and $T = 70$ nm. Calculation by the RCWA method.

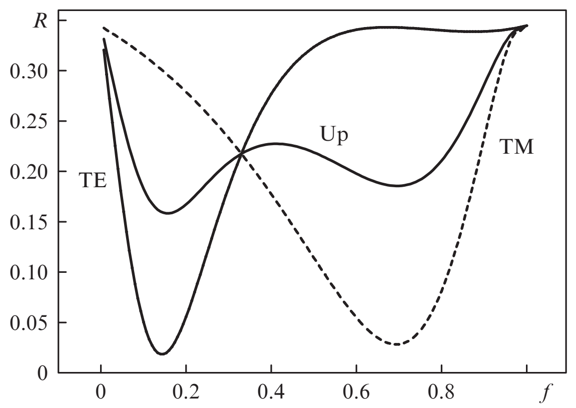

Figure 4. Dependences of the reflectance R on the fill factor f for TE and TM polarisations and unpolarised light Up at $d = 100$ nm, $\theta = 0$ and $T = 70$ nm. Calculation by the RCWA method.

4. Comparison and discussion of the results

Comparison of the curves in Figs 1, 2 and Figs 3, 4 makes it possible to draw a conclusion about the justification of application of an approximate model for calculating the reflectance for both polarisations in the investigated range of variation of the grating parameters on the silicon surface. In the dependence of the reflectance on the grating depth, the periods and positions of the extrema coincide with an accuracy of ~1%. The values of the minima (~0.12) are different, but this difference in the absolute value is about 0.02 for the minima in TE polarisation and about 0.01 for the minima in TM polarisation, which corresponds to the relative accuracy of coincidence of several tens of percent. The reflectance maxima (~0.35), equal to the reflectance for a smooth silicon surface, coincide with an accuracy of about 1% for the two methods of calculation.

In the dependences of the reflectance on the fill factor $R(f)$, the values of the minima and their positions also coincide with a relative accuracy of a few tens of percent and a few percent, respectively. In this case, for TE polarisation $R \sim 0.02$ and $f \sim 0.17$, and for TM polarisation $R \sim 0.03$ and $f \sim 0.72$.

The results obtained are, in our opinion, very interesting given the fact that one of the models (ERI) is based on the interference in a uniform thin film, and the other (RCWA) – on the scattering by a rough surface. It should be noted that the ERI model allows one to clearly interpret a significant reduction in the silicon reflectance at certain grating parameters: the region with a subwavelength grating on the surface acts as a thin quarter-wave antireflection film. Note also that the minimum calculated values of the reflectance, $R \sim 0.02-0.03$, are not limiting and can be reduced by further optimisation of the grating depth and fill factor.

The presented dependences correspond to the case of normal incidence of optical radiation on the surface. However, possible extrapolation of these results to the case of nonzero angles of incidence is not obvious. Thus, we have performed similar calculations of the reflectance from the surface of black silicon at an angle of incidence of optical radiation from 0 to 90°. The obtained result permits the conclusion that the ERI model is also applicable and exhibits the same accuracy as in the case of normal incidence.

Figures 5 and 6 show the angular dependences of the reflectance for TE and TM polarisations at different grating parameters calculated by the RCWA method. The ERI method gives similar results (Figs 7 and 8). An interesting feature here is the nonmonotonic dependence of the reflectance on the angle of incidence for certain values of the grating parameters [curves (*3*) in Figs 5, 7 and curves (*1*) in Figs 6, 8]. The angle, at which the minimum reflectance is achieved, is known in literature as the 'pseudo-Brewster angle' [7]. In the system in question, this effect is an analogue of the Brewster angle effect, but it manifests itself for both TM and TE polarisations and, in contrast to the conventional Brewster angle effect, does not reach zero at the minimum [curve (*4*) in Figs 6, 8]. In this case, this minimum is achieved at angles of incidence from 50° to 60°, i.e., it is displaced to smaller, with respect to the true Brewster angle (75°), values. This is in good agreement with the results of papers [16, 17], in which this effect was first discovered and interpreted for a randomly rough dielectric surface, but only for TM polarisation. As can

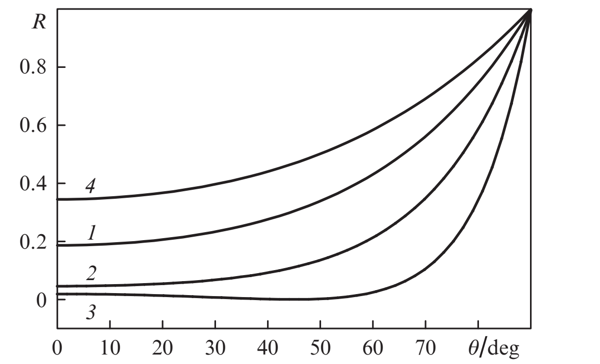

Figure 5. Dependences of the reflectance R for TE polarisation on the angle of incidence θ at $f = 0.15$, $T = 70$ nm and $d =$ (*1*) 50 nm, (*2*) 75 nm and (*3*) 100 nm; curve (*4*) shows the results at $d = 0$. Calculation by the RCWA method.

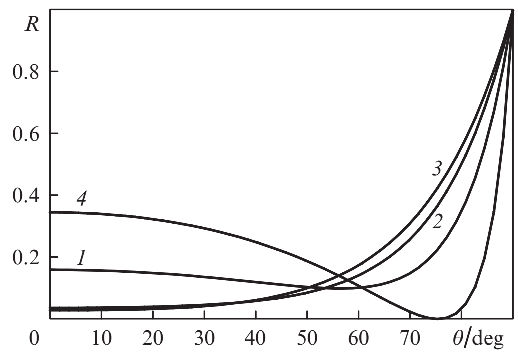

Figure 6. Dependences of the reflectance R for TM polarisation on the angle of incidence θ at $f = 0.70$, $T = 70$ nm and d = (*1*) 50 nm, (*2*) 75 nm and (*3*) 100 nm; curve (*4*) shows the results at $d = 0$. Calculation by the RCWA method.

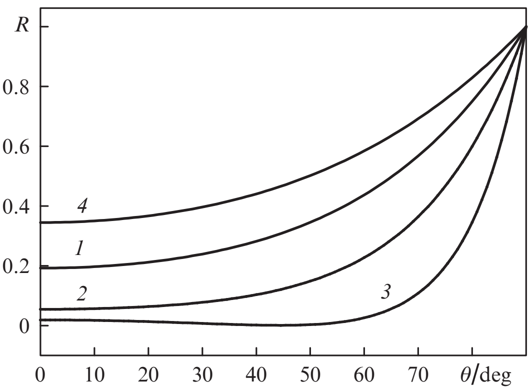

Figure 7. Dependences of the reflectance R for TE polarisation on the angle of incidence θ at $f = 0.15$, $T = 70$ nm and d = (*1*) 50 nm, (*2*) 75 nm and (*3*) 100 nm; curve (*4*) shows the results at $d = 0$. Calculation by the ERI method.

be seen from the presented dependences, unlike conventional Brewster angle, the pseudo-Brewster angle under certain grating parameters may be absent for both polarisations. On the whole, all this indicates the prospects of using the angular dependences of the reflectance to characterise sub-wavelength nanostructures of these type, including technological diagnostics in real time.

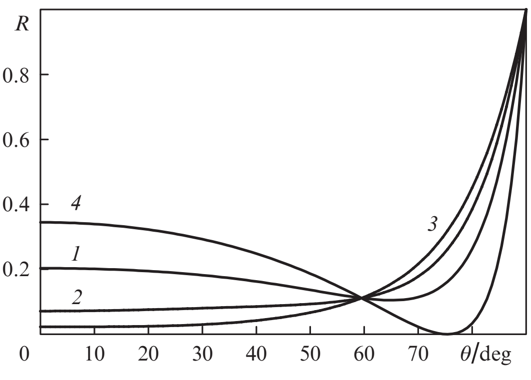

Figure 8. Dependences of the reflectance R for TM polarisation on the angle of incidence θ at $f = 0.70$, $T = 70$ nm and d = (*1*) 50 nm, (*2*) 75 nm and (*3*) 100 nm; curve (*4*) shows the results at $d = 0$. Calculation by the ERI method.

Of course, good agreement between the calculation results by both methods will inevitably be violated if the grating period is increased. At its certain values the changes in the field of an optical wave at distances of the order of the period can no longer be regarded small, which makes the averaging procedure incorrect. The most common quantitative criterion is given in [18]:

$$2\pi|\tilde{n}|T/\lambda_0 \ll 1. \qquad (14)$$

This gives $T \ll 50$ nm and, at first glance, contradicts our results which show that the ERI method gives good accuracy already starting with $T \sim 100$ nm. However, as pointed out by Rytov [18], this criterion is not a necessary condition and in some instances may be replaced by a less rigorous one. It can be assumed that this takes place in our case.

In order to assess the limiting values of the grating period, for which it is still possible to use the ERI method, we have investigated the dependence of the reflectance on the grating period by the RCWA method. The obtained results suggest the possibility of applying the ERI method to calculate the system in question at $T \lesssim 100$ nm.

As an illustration, Fig. 9 shows the dependence of the reflectance on the grating period for TE polarisation at $f = 0.5$ and $d = 55$ nm. It is easy to see that when the period is changed from 0 to 150 nm, the calculated reflectance increases by 50%, from 0.12 to 0.18, and when the period is changed from 0 to 200 nm, the reflectance increases by more than 100%, from 0.12 to 0.26.

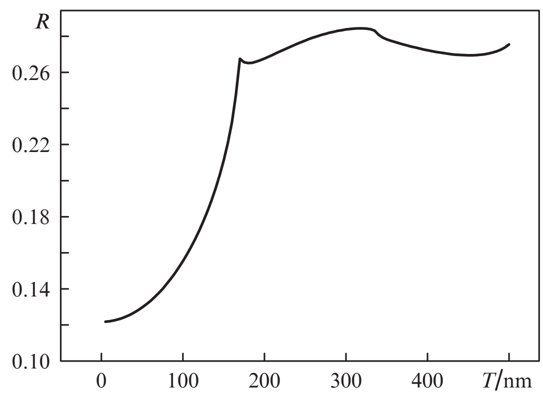

Figure 9. Dependence of the reflectance R for TE polarisation on the grating period T at $d = 55$ nm and $f = 0.5$. Calculation by the RCWA method.

The foregoing suggests that the reflective properties of black silicon are mainly determined by the depth of the relief and the fill factor. The shape of the relief also exerts an influence, but indirectly, through the gradual change in the fill factor over the depth. Nevertheless, we do not rule out the fact that the shape of the relief, such as pointed grating lines, can also play an independent role. This requires a separate study, which we plan to implement in the future, along with the experimental verification of the presented results.

In general, the results and the analysis show that in the range of changes in the grating period from 50 to 100 nm, the calculation of the reflectance of optical radiation from the black silicon surface by both methods yields to similar results. Consequently, the ERI method in conjunction with the

RCWA method may be recommended to calculate and optimise the properties of this material.

5. Conclusions

The results of the simulation of the reflectance of visible light from a sub-wavelength grating with a rectangular profile on the surface of the silicon lead to the following conclusions.

1. Calculation by the ERI and RCWA methods give similar results at grating periods less than 100 nm.

2. A grating with a rectangular profile reduces the reflectance of the polarised light down to ~ 1% at an appropriate choice of the parameters.

3. At a fixed grating period the reflectance is a periodic function of the grating depth, whose period significantly depends on the polarisation of incident light. At the maximum the reflectance is equal to the reflection coefficient for a smooth silicon surface.

4. At a fixed depth of the grating the reflectance is a function of the fill factor (duty cycle). In the first approximation, the corresponding curves for TE and TM polarisations are mirror-symmetric.

5. A grating on a silicon surface leads to a decrease in the pseudo-Brewster angle and the contrast. At certain grating parameters, this effect for both polarisations disappears. At the same time, in contrast to the conventional Brewster effect, the effect of the pseudo-Brewster angle can manifest itself for both polarisations.

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