



Modal analysis of the quasi-resonant extinction ratio enhancement in the amorphous silicon wire grid polarizer

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ABSTRACT

The previously discovered effect of quasi-resonant enhancement of the extinction ratio in an amorphous silicon wire polarizer is investigated using the Bloch wave approach and the modal method. Effective indices of grating modes, modal fields and transmission coefficients were numerically evaluated and our prior hypothesis of destructive interference of lower order grating modes as a mechanism for the enhancement of the extinction ratio was confirmed. Using the numerical optimization, we showed that the quasi-resonance wavelength can be tuned by changing the parameters of the grating structure.

1. Introduction

Wire grid polarizers (WGP) are known as a promising alternative to traditional optical polarizers due to their inherently compact planar structure and reasonably good optical performance [1–3]. The undoubted advantage of WGP is their compatibility with modern thin-film technology which is a key technology in the production of electronic and optical integrated circuits. Today wire grid polarizers are already being used in various optical devices [4–6] and the advantages of this technology are clearly visible.

Interest in to the amorphous silicon nanowire grid polarizers is primarily due to their possible application in UV band (300–400 nm). S. Kroker et al. in Ref. [3] and T. Weber et al. in Ref. [7] investigated the spectral characteristics of this kind of polarizers in the form of parallel ridges of amorphous silicon fabricated on a quartz substrate (Fig. 1). The maximum calculated extinction coefficient of about 10^3 in the vicinity of the wavelength of 400 nm was reported. In our paper [8] where we numerically studied the performance of amorphous silicon nanowire polarizer having different parameters, we found an interesting feature in the spectral dependencies of the extinction coefficient. A very sharp peak near the 378 nm wavelength with an extinction coefficient of about 10^6 was found for some specific structure parameters. We called the effect a quasi-resonance and interpreted as dissipative-interference one. First of all, the term “quasi-resonance” indicates the similarity of the extinction ratio graph to typical resonant dependences in the classical sense [9]. At the same time, it points out that the characteristics of the effect under study do not fully match the classical definition of resonance, i.e., sharp increase in the amplitude of physical oscillations at a

certain frequency. Nevertheless, resonance and interference as physical phenomena are closely related, and sometimes equivalent, as, for example, in the case of the classical Fabry-Perot resonator. Thus, the use of the term “quasi-resonance” for the effect under study is, in our opinion, reasonable.

The extinction ratio (ER) is defined as the ratio of the transmittances for two polarizations of the incident radiation:

$$ER = \frac{T_{TM}}{T_{TE}}, T_{TM} = \frac{I_{TM}}{I_{TM}^0}, T_{TE} = \frac{I_{TE}}{I_{TE}^0} \quad (1)$$

where T_{TM} and T_{TE} are the transmission coefficients for TM and TE polarizations, I_{TM} and I_{TE} are the intensities of radiation with TM and TE polarizations at the output of the polarizer, I_{TM}^0 and I_{TE}^0 are the corresponding input intensities of optical radiation. We call polarization TE when the grating vector is perpendicular to the electric vector of the incident wave, and TM if the grating vector is perpendicular to the magnetic vector of the incident wave. The change in the extinction ratio may occur as a result of a change in either of the two polarization transmittances. As shown in Ref. [8], a sharp increase in the extinction ratio is a consequence of the same sharp decrease in the transmittance of the polarizer at TE polarization (Fig. 2). This conclusion is supported by the fact that the transmission coefficient at the TM polarization, as well as the reflection coefficients at both polarizations, does not show any peculiarities in the vicinity of the quasi-resonance conditions. The quasi-resonance is achieved with the following main parameters of the structure: incident radiation wavelength $\lambda = 378$ nm, grating depth $h = 80$ nm, period $\Lambda = 120$ nm, filling factor $f = 0.5$, refractive index of

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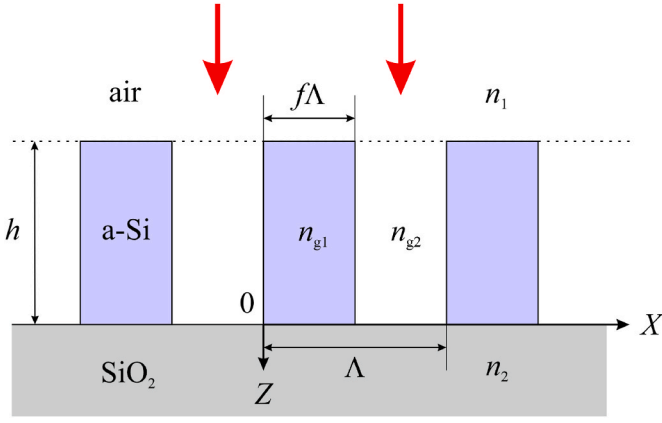


Fig. 1. Wire grid polarizer.

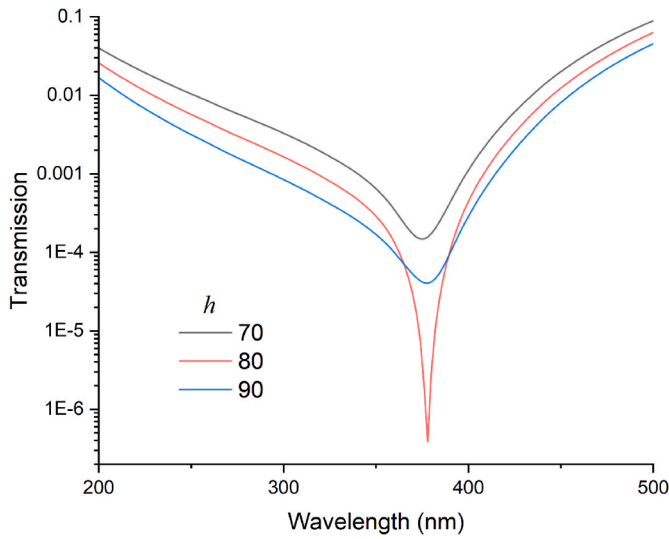


Fig. 2. Dependence of the TE-polarization transmission on the wavelength at different grating depths.

amorphous silicon $n_{g1} = 4.070 + i \cdot 2.499$ [10], refractive index of substrate $n_2 = 1.457$ [11] (at the given wavelength). These parameters will be further used for all calculations. We took into account the material dispersion in our calculations when varying the wavelength.

Taking into account the nonmonotonic and sharp dependence of the transmittance on the grating depth, we proposed a qualitative explanation of the revealed effect as a quasi-resonant mode interference [8]. In this approach, the individual elements of the array, that is, the ridges and the gaps between them, are considered as separate optical “waveguides”. The grating, in this approach, is treated as a periodic system of waveguides with two adjacent “waveguides” on the period of the grating, silicon with a width $f\Lambda$ and a hollow one with a width $(1-f)\Lambda$. Within this model the polarization dependence for this structure is a consequence of a significant difference in the damping coefficients of the waveguide modes excited at the TE and TM polarizations of the incident radiation. It is this difference that makes the main contribution to the value of the extinction ratio outside the region of the quasi-resonance. On the other hand, in the vicinity of the quasi-resonance conditions, the transmittance at TE polarization decreases further due to the destructive interference of radiation at the output of adjacent vacuum and silicon waveguides. However, these qualitative arguments were really just a hypothesis that needed quantitative proof.

Thus, the aim of this work is to quantitatively analyze the phenomena occurring in an amorphous silicon wire polarizer in the vicinity of

quasi-resonance using rigorous methods to confirm the previously stated hypothesis.

The work is structured as follows:

In the second section we present the basic mathematical expressions that describe the optical fields in the structure of the polarizer based on the Bloch waves approach.

In the third section we discuss results of the corresponding numerical simulation.

In the fourth section we formulate the conclusions.

2. Basic analytical relationships and calculation method

To get a quantitative explanation of the quasi-resonance effect, it is necessary to analyze the structure of the optical fields in the structure under study. For this purpose, following [12–14], we used the modal method. In Ref. [12] it was pointed out that the modal method is especially convenient for understanding the interference effects in lamellar diffraction gratings including nanowire polarizers. Within this approach, the optical fields inside the grating are treated as a combination of modes, which are eigen solutions of Maxwell’s equations for the periodic distribution of dielectric permittivity along the X axis. Since the structure under consideration is periodic, each mode is a Bloch wave, and hence the properties of optical fields are determined by the fundamental properties of such waves [15].

A plane wave is incident on the grating at an angle θ_0 with respect to the Z axis. Electric $\mathbf{E}$ and magnetic $\mathbf{H}$ components of the incident optical field can be represented as:

$$\begin{bmatrix} \mathbf{E}_i(x, z, t) \\ \mathbf{H}_i(x, z, t) \end{bmatrix} = \begin{bmatrix} \mathbf{E}_0 \\ \mathbf{H}_0 \end{bmatrix} \exp(ik_x x) \exp(ik_z z) \exp(-i\omega t) \quad (2)$$

where

$$k_x = k_0 n_1 \sin \theta_0, \quad k_z = k_0 n_1 \cos \theta_0 \quad (3)$$

n_1 is the refractive index of the upper medium;

$k_0 = \frac{2\pi}{\lambda}$ is the wavevector in vacuum; θ_0 is the angle of incidence; It is known that in the case of periodic dependence of dielectric permittivity on the coordinate x , the solution for the total diffraction field has the following form, according to the Floquet-Bloch theorem:

$$\begin{bmatrix} \mathbf{E}(x, z) \\ \mathbf{H}(x, z) \end{bmatrix} \exp(iK_B x) \exp(-i\omega t) \quad (4)$$

where functions $\mathbf{E}(x, z)$ и $\mathbf{H}(x, z)$ are periodic in the x -direction,

K_B is the Bloch vector, which is determined by the projection of the wave vector of the incident wave k_x onto the X axis, Λ is the grating period.

Due to the periodicity of the functions $\mathbf{E}(x, z)$ and $\mathbf{H}(x, z)$ they can be expanded in a Fourier series, which leads to the representation of diffraction fields in the regions of space above and below the grating in the form of a Rayleigh-Fourier expansion:

$$\begin{bmatrix} \mathbf{E}_d(x, z) \\ \mathbf{H}_d(x, z) \end{bmatrix} = \begin{cases} \sum_{m=-\infty}^{\infty} \begin{bmatrix} E_m^1 \\ H_m^1 \end{bmatrix} \exp(ik_{xm} x) \exp(ik_m^1 z), \\ \sum_{m=-\infty}^{\infty} \begin{bmatrix} E_m^2 \\ H_m^2 \end{bmatrix} \exp(ik_{xm} x) \exp(ik_m^2 z) \end{cases},$$

$$k_{xm} = k_x + \frac{2\pi m}{\Lambda}, \quad k_m^j = \sqrt{\omega^2 \mu_0 \epsilon_j - k_{xm}^2}, \quad j = 1, 2.$$

The values of index j 1 and 2 identify the field above and below the grid, respectively.

As for the field in the grating region, it is represented as the sum of the grating modes:

$$\begin{bmatrix} \mathbf{E}(x, z) \\ \mathbf{H}(x, z) \end{bmatrix} = \sum_{q=0}^{\infty} \begin{bmatrix} \mathbf{E}_q(x) \\ \mathbf{H}_q(x) \end{bmatrix} \left[a_q^+ \exp(-i\beta_q z) + a_q^- \exp(i\beta_q z) \right]$$

where for a mode of order q , β_q is the propagation constant, a_q^+ and a_q^- are the amplitudes of waves propagating in different directions of the Z axis and $\begin{bmatrix} \mathbf{E}_q(x) \\ \mathbf{H}_q(x) \end{bmatrix}$ is the lateral distribution of the mode field [12].

The mode fields in each grating region are represented as a sum of plane waves as the dielectric permittivity is constant inside the region. Using periodic boundary conditions, it is possible to obtain the dispersion equations for the effective refractive indices of the TE and TM modes [13]:

$$f_{TE}(n^{*2}) = \cos k_{g1} d_1 \cdot \cos k_{g2} d_2 - \frac{1}{2} \left(\frac{k_{g1}}{k_{g2}} + \frac{k_{g2}}{k_{g1}} \right) \sin k_{g1} d_1 \cdot \sin k_{g2} d_2 = \cos k_x \Lambda \quad (5)$$

$$f_{TM}(n^{*2}) = \cos k_{g1} d_1 \cdot \cos k_{g2} d_2 - \frac{1}{2} \left(\frac{\epsilon_{g2} k_{g1}}{\epsilon_{g1} k_{g2}} + \frac{\epsilon_{g1} k_{g2}}{\epsilon_{g2} k_{g1}} \right) \sin k_{g1} d_1 \cdot \sin k_{g2} d_2 = \cos k_x \Lambda \quad (6)$$

$$k_{g1} = k_0 \sqrt{n_{g1}^2 - n^{*2}}, k_{g2} = k_0 \sqrt{n_{g2}^2 - n^{*2}}$$

$$n^* = \beta/k_0$$

Here, is the effective refractive index of the mode, k_x is the x component of wave vector of the incident wave, n_{g1} and n_{g2} are the refractive indices of amorphous silicon and the free gap, respectively, $d_1 = f\Lambda$, $d_2 = (1 - f)\Lambda$. Below we focus on the case of normal incidence, when the right-hand side of the Eqs. (5-6) becomes equal to one.

3. Analysis of the calculation results and quasi-resonance as a consequence of mode interference

The approach shown above and developed in Refs. [12–14] provides the way for clear physical explanation and understanding of the quasi-resonance. The field distribution of the individual modes and their contribution to the transmittance can be calculated analytically. However, this requires a large number of analytical transformations, and the final expressions are difficult to analyze because they are cumbersome. Therefore, to calculate the characteristics of individual modes we used the computer program MC Grating [16] which employs RCWA (Rigorous Coupled Wave Analysis) [17] and TMM (True Modal Method) [13] methods. We verified that for this structure the analytical approach [12,14] and the numerical approach based on the RCWA and TMM methods give the same results. In particular, we got the same sets of effective refractive indices of modes and mode fields that are presented in Table 1 and Fig. 3.

The effective refractive indices presented in Table 1 are exact solutions given by computer program MC Grating at the quasi-resonance condition. The same solutions can be obtained from Eqs. (5-6) as the

Table 1

Effective refractive indices for the low order TE and TM modes of the polarizer at quasi-resonance.

q (TE)	$\text{Re}[n^*]$	$\text{Im}[n^*]$	q (TM)	$\text{Re}[n^*]$	$\text{Im}[n^*]$
0	3.49584	2.6341	0	1.10138	0.197139
1	0.571442	2.1942	1	3.18545	3.13907
2	2.00936	3.20225	2	0.0986908	2.8594
3	0.699424	5.75154	3	1.72834	5.74901
4	0.91819	5.9472	4	0.0231929	6.1504
5	0.511009	9.1228	5	1.11326	9.00567
6	0.570683	9.7552	6	0.00975594	9.34862
7	0.392609	12.364	7	0.822106	12.2491
8	0.417116	12.3855	8	0.00553543	12.5233

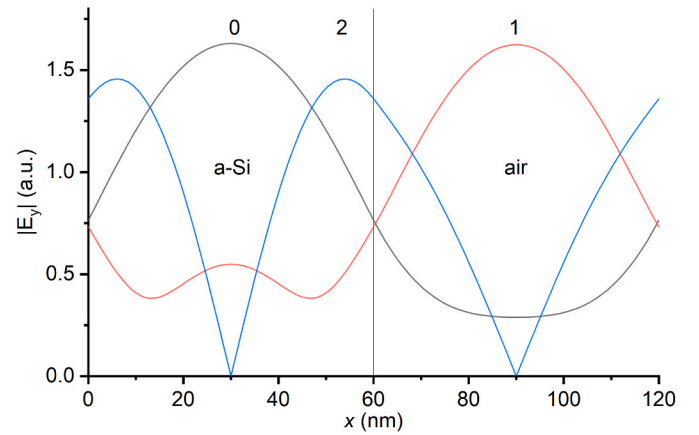


Fig. 3. Field distributions for the lower order TE grating modes.

intersection points of the real and imaginary parts of the equations, which is illustrated for the case of TE polarization in Fig. 4. This graphical approach allows for a better understanding of the modal structure.

A useful additional technique that helps to understand the general features of these solutions is the analysis of the dispersion function $f(n^{*2})$ without taking into account the imaginary component of the refractive index n_{g1} [12,14]. In this case, the analysis can be greatly simplified while the results are close to the real-world case, when the ridges are made of material having some absorption. Fig. 5 shows the dependence of the function f_{TE} on the square of the effective refractive n^{*2} . The solutions of the dispersion equation are given by the intersection points of the function $f(n^{*2})$ graph with the horizontal line corresponding to the right side of the equation.

The effective refractive index for a Bloch wave is determined by the Bloch vector and hence the angle of incidence of the optical radiation on the polarizer. This isolates a discrete set of modes that can be excited at a given angle of incidence from the continuous spectrum of possible eigen solutions. Due to the structure periodicity the regions of possible

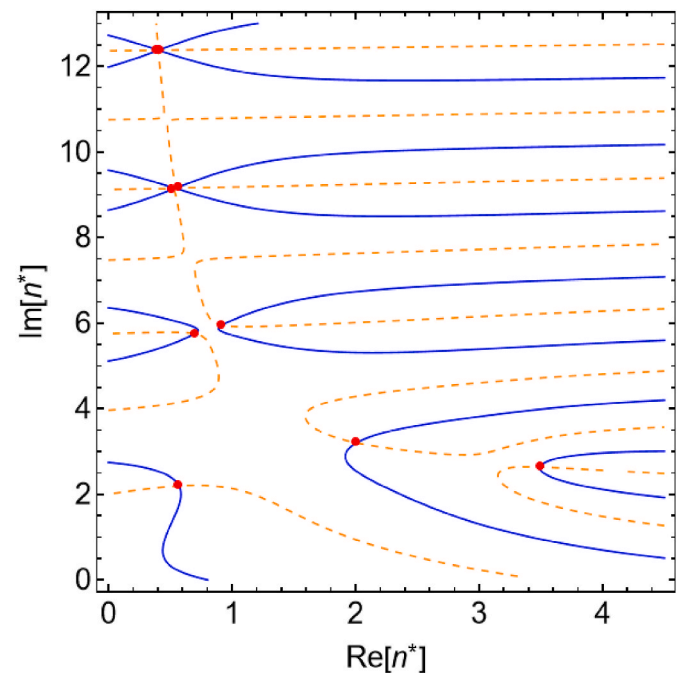


Fig. 4. Graphical solution of Eq. (5) at quasi-resonance. Solid line – real part of the equation, dashed line – imaginary part. Grating modes are shown as circles.

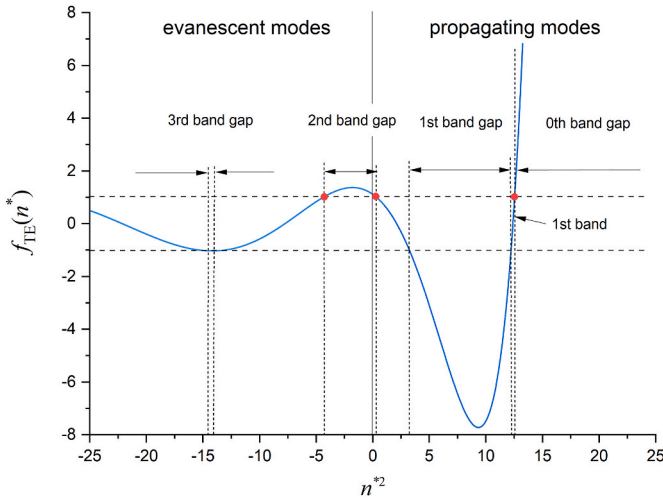


Fig. 5. Function $f_{TE}(n^*)$, calculated for the lossless grating. $n_{g1} = 4.07$, $n_{g2} = 1$, $d_1 = d_2 = 60$ nm, $\lambda = 378$ nm. Grating modes are shown as circles.

continuous changes of the effective refractive index n^* (bands) are separated by band gaps. Within the band gaps Bloch vector has a complex value and the corresponding Bloch wave amplitude exponentially decreases along the X axis [15]. Therefore, such a wave cannot be excited by a plane wave incident from the upper medium. Inside every band there is a single mode corresponding to the particular angle of incidence with a real Bloch wavevector and in our case of normal incidence the excited Bloch waves are located exactly at the band gap boundaries, this case is also known as “critical” [18].

Three regions of n^{*2} values can be distinguished in Fig. 5. If $n^{*2} > n_1^2$ Eq. (5) has no real solutions and this region can be referred as zero-order band gap [18]. Two solutions exist in the region $0 \leq n^{*2} \leq n_{g1}^2$ and correspond to the Bloch waves having real n^* thus propagating along the Z axis. In the region $n^{*2} < 0$, function f_{TE} becomes quasi-periodic, its extrema exceed unity in absolute value [12] and the possible solutions correspond to Bloch waves with imaginary n^* exponentially decreasing in the direction of the Z axis (evanescent). In case of normal incidence, only modes with the Bloch vector at the boundaries of band gaps of even order ($K_B \Lambda = \pm 2\pi m$, $m = 0, 1, 2$) are excited. The number of zeros in the amplitude profile of the mode in lossless case is equal to the order of the band gap. According to Fig. 5, the real parts of the effective refractive index of the 0th and first TE-mode are approximately 3.54 and 0.57, respectively, and the imaginary parts for the 2nd, 3rd, and 4th TE modes are 2.1, 5.53, and 5.65, which corresponds well to Table 1 data except for the 2nd mode, and the pair character of higher order modes is clearly visible, one of the modes is even, and the other is odd with respect to the vertical axes of symmetry passing through the middle of the grating regions [12]. The paired nature of the higher modes, characterized also by their progressive convergence with increasing mode number, is also clearly visible on the graph of the exact solutions of the dispersion equation (Fig. 4).

The main contribution to the transfer of optical energy through the nanowire grating is made by the TM_0 mode, since the imaginary part of its effective refractive index is an order of magnitude smaller than the imaginary part of the effective refractive index for the TM_1 mode. The real part of the effective refractive index of the TM_0 mode is close to the refractive index of the hollow gap. Note that, as pointed out in Ref. [12], a good estimate for the effective refractive index for the TM_0 mode is given by the Sommerfeld-Zenneck formula for the propagation constant of a surface metal-dielectric plasmon:

$$n^* = \sqrt{\frac{\epsilon_{g1}\epsilon_{g2}}{\epsilon_{g1} + \epsilon_{g2}}}$$

This gives a good estimate for the effective refractive index $0.99 +$

$0.018i$ and reaffirms the analogy of the TM_0 mode field with the surface plasmons fields [12].

As can be seen from the data presented in Table 1 and Fig. 3, the two modes TE_0 and TE_1 with the lowest attenuation, which make the main contribution to the transfer of optical energy through the nanowire grating at TE polarization, can be called the nanowire ridge mode and the hollow gap mode. These modes are characterized by complex effective refractive indices, the real parts of which approximately correspond to the real part of the refractive index of amorphous silicon and air respectively, and the imaginary parts are approximately the same. Higher order modes have a significantly higher losses and thus do not affect the transmission of the polarizer. Moreover, the TE_2 mode has an antisymmetric profile and thus can't be excited at the normal incidence at all and hence can't contribute to the transmission.

Fig. 6 presents the calculated dependence of the structure transmission on the thickness of the grating h . Our implementation of the modal method in MC Grating program allowed us to calculate the contribution of different structure modes to the total transmission separately. It can be seen that under quasi-resonance conditions the contribution to the energy transfer is approximately the same for the first two TE modes and their phase relative to each other is shifted by π , which leads to destructive interference. We also confirmed that the contribution of all other modes is too small to be seen on the graph. Thus, it can be concluded that the destructive interference of TE_0 and TE_1 modes near the quasi-resonance position leads to minimal transfer at the TE polarization which in turn is responsible for the extinction ratio increase. A rough estimation of the phase difference $\Delta\phi$ between the two modes based on the real parts of the corresponding effective refractive indices gives approximately 1.2π . Here it should be noted that the conversion of modes of the grating into plane waves in neighboring semi-infinite media results in an additional phase shift, which was taken into account in numerical calculations. At TM polarization, no peculiarities in the transmission behavior in the vicinity of the quasi-resonance point are observed.

Thus, we see that the dissipative-interference mechanism of extinction ratio enhancement put forward earlier on the basis of qualitative arguments is in perfect agreement with accurate calculations of the fields in the nanowire polarizer. Mode interference could play a significant role in other types of microdevices. For example, there are recent papers dealing with it in various magneto-optical devices operating in the terahertz range [19–21].

Understanding the nature of the quasi-resonance effect allows us to suggest the possibility of controlling this effect by changing the geometric parameters of the polarizer, which should lead to a change in the

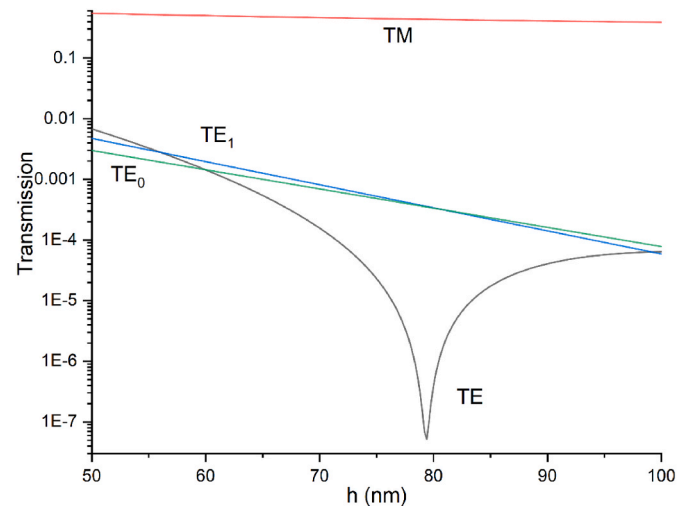


Fig. 6. Polarizer transmission for TE and TM polarizations as a function of grating depth h .

amplitude-phase and dispersion characteristics of excited modes, and hence the spectral characteristics of the nanowire polarizer. A change in the wavelength of the incident optical radiation leads to a violation of the quasi-resonance condition, but the mode model suggests that it can be tuned again by changing the geometric parameters of the grating. To test the validity of this assumption, we changed the wavelength to $\lambda = 400$ nm and then minimized the transmission at this wavelength by adjusting the geometric parameters of the grating. The result was a shifted quasi-resonance with an extinction ratio of 10^7 at a grating depth of 91 nm, a period of 124.1 nm, and a filling factor of 0.322, which demonstrated that the quasi-resonance position can be tweaked.

4. Conclusions

We have analyzed the phenomenon of quasi-resonance in thin-film amorphous silicon nanowire polarizers. The analysis is based on the Bloch wave theory and numerical calculations. As a result, the previously proposed hypothesis about the dissipative-interference nature of the effect was confirmed, namely, it was shown that the effect is a consequence of destructive interference of the first two TE modes of the nanowire polarizer. The possibility of shifting the resonant wavelength by adjusting the geometrical parameters of the nanowire polarizer is demonstrated. Thus, the effect can be used to design a WGP with better extinction ratio at a given wavelength.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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