CHIN. PHYS. LETT. Vol. 31, No. 6 (2014) 064205

Modeling of Fano Resonance in High-Contrast Resonant Grating Structures *

HU Jin-Hua(胡劲华), HUANG Yong-Qing(黄永清)**, REN Xiao-Min(任晓敏), DUAN Xiao-Feng(段晓峰), LI Ye-Hong(李业弘), WANG Qi(王琦), ZHANG Xia(张霞), WANG Jun(王俊)

State Key Laboratory of Information Photonics and Optical Communications, Institute of Optical Communication and Optoelectronics, Beijing University of Posts and Telecommunications, Beijing 100876

(Received 24 December 2013)

A new model is presented for Fano resonance in resonant grating structure based on the temporal coupled mode theory. By using this model, the reflection spectrum can be reproduced with the information of eigenmode of the structure, which can be numerically calculated by the finite element method. Therefore, the eigenmode plays a key role in determining the profile of the line shape of the Fano resonance in the resonant grating structure. When the space of two grating modulations is decreased, the line shape experiences a significant change. Such a drastic change can be attributed to the increase of quality factor of the eigenmodes. Thus, our model not only provides a simple and intuitive understanding on the mechanism of Fano resonance, but it also offers a convenient way to engineer the line shape of the Fano resonance. The proposed model can be used in many applications, such as biosensors, optical filters, and optical switchers.

PACS: 42.79.Dj, 42.25.−p, 42.60.Da DOI: 10.1088/0256-307X/31/6/064205

Subwavelength gratings have attracted considerable research interest in recent years due to their unique characteristics. These gratings are widely used as broadband refection mirrors,[1] wide band polarizer,[2] optical sensors,[3] and optical couplers.[4] A new type of subwavelength grating structure that is fully surrounded by low index media, which is called high-contrast grating (HCG),[5] has recently been proposed. HCG has been employed to realize broadband reflection. Moreover, HCG can be also used as an optical resonator with Fan resonance.[6] Fano resonance generally originates from the interference between a coherent background pathway and a resonance-assisted pathway.[7] A large number of research works have been reported on Fano resonance in HCG. For example, Zhou *et al.* designed and demonstrated a GaAs-based high quality resonator to achieve high-Q value using the Fano resonance in subwavelength HCG.[8] Karagodsky *et al.* presented a simple analytic method to explain the multimode Fabry-Pérot resonance mechanism in resonant HCG.[9] Ahmed *et al.* provided a coupled mode theory to design and analyze a high-Q HCG resonator with Fano resonance.[10] Wu *et al.* achieved surface-emitting lasers using the Fano resonance based on GaN-based high contrast grating.[11]

To our knowledge, Fano resonant grating structures are usually designed by using rigorous electromagnetic simulation methods.[12−14] Most of these simulation methods tend to have a complicated mathematical nature that lacks intuitive physical understanding of the Fano resonance mechanism. Although good simulation results can be obtained, the understanding is unclear enough and time consuming. Here, a new model is proposed based on temporal coupled-mode theory (TCMT).[15] It can quickly simulate the linear region, which is most important for a Fano resonance. Since the proposed method can represent the physical nature, the Fano resonance can be more clearly understood and the devices can be more easily designed. This method may be beneficial to the study of the Fano resonance in HCG. We found that the reflection spectrum of the resonant grating structure can be reasonably reproduced by using TCMT with the information of eigenmode of the grating structure.[16,17] Furthermore, we also find that the line shape of Fano resonance is directly determined by the eigenvalue of the mode. Therefore, our model provides a simple and direct method to engineer the line shape of Fano resonance by engineering the eigenmode of the structure. It may open up a pathway to design Fano-resonant grating structures for potential applications, like optical filters, and biosensing, among others.

In this model, the TCMT method is used to analyze the Fano-resonant properties of the resonant grating structure. The Fano resonance transmission or reflection spectra can be calculated based on TCMT and the eigenmode of the resonant grating structure. For

*Supported by the National Basic Research Program of China under Grant No 2010CB327600, the National Natural Science Foundation of China under Grant Nos 61020106007 and 61274044, the Natural Science Foundation of Beijing under Grant No 4132069, the Program of Key International Science and Technology Cooperation Projects under Grant No 2011RR000100, the Fundamental Research Funds for the Central University under Grant No 2011RC0403, the 111 Project of China under Grant No B07005, the Specialized Research Fund for the Doctoral Program of Higher Education of China under Grant No 20130005130001, and the Program for Changjiang Scholars and Innovative Research Team in University under Grant No IRT0609.

**Corresponding author. Email: yqhuang@bupt.edu.cn

© 2014 Chinese Physical Society and IOP Publishing Ltd

simplicity, in our model two conditions are assumed: one is that the structure is a symmetric single-mode resonator; the other is that the materials in the structure have no intrinsic absorption loss.

We start our simulation with the eigenmode in the resonant grating structure using the finite element method (FEM). In this simulation, we choose a period of the resonant grating structure as a unit cell, where Floquet-periodic boundary conditions are applied for lateral boundaries and scattering boundary conditions for upper and lower boundaries.[18] The eigenmode of the resonant grating structure is then obtained; with complex values for a normalized parameter $N = N_{\text{real}} - i^* N_{\text{imag}}$. We can thus obtain an eigenvalue. According to this calculated eigenvalue, we can find the central resonance frequency ω_0 and total radiative quality factor q_0 of the single-mode resonant grating structure as follows:[19]

$$\begin{aligned} \omega_0 &= N_{\text{real}}, \\ q_0 &= N_{\text{real}}/2N_{\text{imag}}, \end{aligned} \tag{1}$$

where N_{real} and N_{imag} are the real and imaginary parts of the eigenvalue of the eigenmode in the resonant grating structure, respectively. We also obtain the value of total decay rate τ by using Eq. (7) and relation $\tau = 2q_0/\omega_0$.[20]

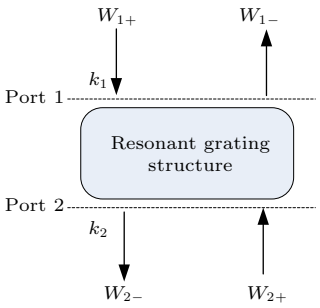


Fig. 1. (Color online) Schematic diagram of the two-port resonance theory model.

The resonant grating structure can be viewed as a symmetric single-mode two-port system based on the temporal coupled mode theory, as shown in Fig. 1. In the TCMT method, the coupled-mode equations can be written as follows:[15]

$$\frac{d\psi}{dt} = \left(j\omega_0 - \frac{1}{\tau}\right)\psi + \begin{pmatrix} k_1 & k_2 \end{pmatrix}^* \begin{pmatrix} W_{1+} \\ W_{2+} \end{pmatrix}, \tag{2}$$

$$\begin{pmatrix} W_{1-} \\ W_{2-} \end{pmatrix} = C \begin{pmatrix} W_{1+} \\ W_{2+} \end{pmatrix} + \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} \psi, \tag{3}$$

where ψ is the resonance-mode amplitude, ω_0 and τ are the central frequency and total decay rate of the resonance, respectively; W_{1+} and W_{2+} are the amplitudes of incoming waves; W_{1-} and W_{2-} are the amplitudes of outgoing waves; and k_1 and k_2 are coupling coefficients at the two ports. We can derive $k_1^* k_1 = k_2^* k_2 = 1/\tau$ based on energy conservation law and time-reversal symmetry. In addition, the scattering matrix C of the direct transport process is expressed by

$$C = e^{i\phi} \begin{pmatrix} r & jt \\ jt & r \end{pmatrix}, \tag{4}$$

where ϕ is the phase factor; r and t are the amplitude reflection and transmission coefficient, respectively. In the direct transport process, r and t satisfy the relation $r^2 + t^2 = 1$ (r and t are both real number). According to the above discussion, we can obtain the transmission or reflection spectra of the resonator as follows:

$$R = \frac{r^2(\omega - N_{\text{real}}) + t^2 N_{\text{imag}} \mp 2rt(\omega - N_{\text{real}})N_{\text{imag}}}{(\omega - N_{\text{real}})^2 + N_{\text{imag}}^2}. \tag{5}$$

To calculate the amplitude reflection r and transmission coefficient t, we can consider the resonant grating structure as a uniform slab waveguide with the same thickness t_{g} and effective refractive index N_{eff}. According to the effective media theory, the effective refractive index N_{eff} can be obtained based on the relation[21]

$$N_{\text{eff}} = ((1 - ff)^2 n_{\text{L}}^2 + n_{\text{H}}^2 ff)^{\frac{1}{2}}, \tag{6}$$

where ff is defined as the ratio of the total widths of the high-contrast grating modulations and the period in unit cell. The amplitude reflection r and transmission coefficient t are then obtained by using the slab waveguide theory.[22] According to the above calculation results, we can calculate the reflection spectra of resonant grating structure using Eq. (5).

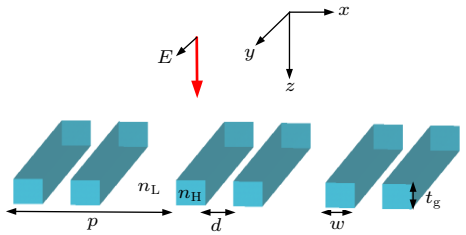


Fig. 2. (Color online) Scheme of the high-contrast resonant compound grating structure. Here, t_{g} is the thickness of the grating layer; p is the grating period; n_{H} and n_{L} are the high and low refractive indexes, respectively; d is the space between two grating modulations; and, w is the widths of the each grating modulation

This proposed model indicates that the Fano resonance of resonant grating structures is governed by the coupling between the incident light and the eigenmode of the grating structures. Unlike typical rigorous methods (i.e., RCWA) for the design of the Fano resonant grating structures, this model has the capability of designing the shape line of Fano resonance by using the eigenmode of the grating structure.

In this work, we present a new high-contrast resonant grating structure, in which each period consists of two grating strips with identical width, as shown in Fig. 2. This grating structure is fully surrounded by the low-index material, which is referred to as high-contrast resonant compound grating (HC-RCG). The light is assumed to be normal-incident TE-polarized plane wave with the electric field parallel to the y direction. The structure is considered to be infinite in the y direction and infinitely periodic in the x direction.

Table 1. Eigenvalues of the TE eigenmode with different spacings.

Spacing (nm)	Eigenvalue
0	$2.493173\times10^{15}-6.756739\times10^{13}i$
10	$2.493653\times10^{15}-4.247039\times10^{13}i$
20	$2.494656\times10^{15}-2.627083\times10^{13}i$
50	$2.496534\times10^{15}-7.424767\times10^{12}i$

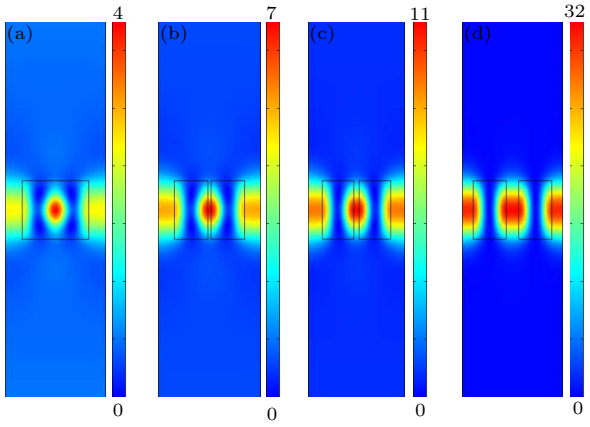


Fig. 3. (Color online) Electric field intensity distributions of the eigenmode mode in different high-contrast resonant compound grating structures with various spacings: (a) $d = 0$ nm, (b) $d = 10$ nm, (c) $d = 20$ nm, (d) $d = 50$ nm.

To demonstrate our proposed model, we will give a simple example, as used in Ref. [6]. We assume the parameters of the HC-RCG structure as follows:[6] $t_{\rm g} = 235$ nm, $p = 380$ nm, $n_{\rm H} = 3.2137$ (e.g., $Al_{0.6}Ga_{0.4}As$), $n_{\rm L} = 1$ (e.g., air), and $w = 125$ nm. In this work, we focus on investigating each HC-RCG structure with different spacing d in unit cells. To obtain the eigenvalue of HC-RCG, we will calculate the eigenvalues of each HC-RCG structure with different spacing d using the FEM method. In our calculations, we choose the different spacings $d = 0$, 10, 20 and 50 nm. These eigenvalues are listed in Table 1. This shows that the real part of the eigenvalues exhibit a small variation with increasing d, while this trend does not hold true for the image part. According to Eq. (1) and Table 1, we can obtain the central resonance frequencies and radiative quality factors of the HC-RCG structure. This shows that the central resonance frequencies of each HC-RCG structure nearly remain unchanged, while the total radiative quality factors of these HC-RCG structures are largely enhanced. This difference indicates that the total radiative quality factors are varied very significantly for HC-RCG with different spacings.

To further understand the physical nature of the eigenmode, we show the electric field intensity distributions of the eigenmodes for different d in each unit cell of the HC-RCG structure using the FEM method, as shown in Fig. 3. We find that the enhanced electric field of the eigenmodes is confined in the slits of the grating modulation in each unit structure. To gain physical insight into the origin of the different electrical field intensity distributions with different HC-RCG structures, the mode confinement factor of the each eigenmode is calculated and can be expressed as

$$\Gamma = \frac{\int\limits_{G} |E_{\rm norm}|^2 dxdz}{\int\limits_{U} |E_{\rm norm}|^2 dxdz}, \tag{7}$$

where G and U represent the integration domain for grating and the unit cell, respectively; $E_{\rm norm}$ represents electrical field intensity distributions of the eigenmodes. In Table 2, the confinement of the eigenmode is evidently enhanced with the increase of spacing d. This finding indicates that we can improve the confinement of the eigenmode by increasing d. This condition enhances the total radiative quality factors in these HC-RCG structures.

Table 2. Confinement factor of the TE eigenmode with different spacings.

Spacing (nm)	Confinement factor
0	0.0392
10	0.0721
20	0.1178
50	0.3602

Finally, we calculate the reflection spectrum of each HC-RCG structure with different spacing d for TE polarization using the model method, as shown in Fig. 4. From Fig. 4, we find that the reflection spectrum shows asymmetric Fano resonance sharp lines with only a single peak, which is associated with the eigenmode of HC-RCG. In Fig. 4, we compare our reflection spectrum with the RCWA simulation results. Consequently, it can be seen that the calculated resonant wavelengths of two simulations agree well with each other in the linear shape region. Our calculation indicates that the profile of line shape of the Fano resonance is mainly determined by the eigenmode in HC-RCG structure. Therefore, the eigenmode provides great convenience for engineering the Fano resonance of resonant grating structure with arbitrary structure parameters. In the other regions, there are differences between the proposed model method and the RCWA method. The fact that our model focuses on the narrow bandwidth of Fano resonance under the single mode condition is responsible for this phenomenon.

In comparison, in the RCWA method, all the Fourier components are involved, so that the whole light fields of HC-RCG are represented. In addition, line width of Fano resonance is decreased by increasing the distance of spacing d in this example, which can be explained by employing the mode confinement of the eigenmode in HC-RCG structure shown in Table 2. Compared with Ref. [23], we provide an HC-RCG structure to control the line width of Fano resonance using the new model method with physical understanding.

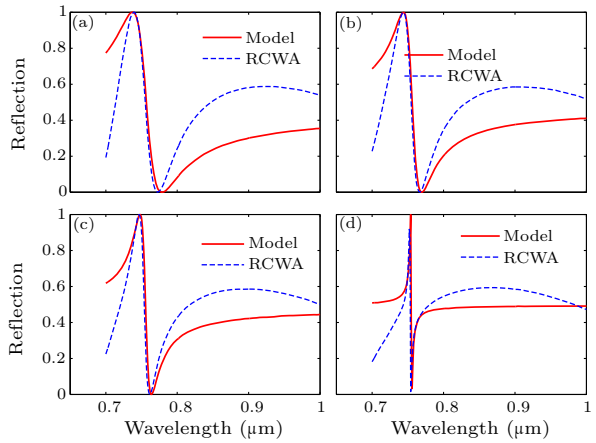


Fig. 4. (Color online) Reflection responses of the high-contrast resonant compound grating structure for the TE polarization with various spacings: (a) $d = 0$ nm, (b) $d = 10$ nm, (c) $d = 20$ nm, (d) $d = 50$ nm.

In summary, we have developed a semi-analytical model for the analysis of high-contrast resonant grating structures and we have investigated the Fano resonance of the HC-RCG structure using the proposed model. We study the effect of the parameters of the HC-RCG structure on the reflection spectral widths and line shape using the eigenmodes of the grating structure. We further understand the nature of Fano resonance in the resonant grating structure. The Fano line shape of the resonant grating structure is attributed to the presence of eigenmodes governed by grating structures. This model provides a new design method to explore new resonant grating structures. The designed HC-RCG structure can be used as an optical sensor, laser mirror, and optical switcher.

References

[1] Mateus C F R, Huang M C Y, Chen L and ChangHasnain C J 2004 *IEEE Photon. Technol. Lett.* **16** 1676
[2] Cao W, Ma J Y and Zhou C H 2012 *Chin. Opt. Lett.* **10** 112301
[3] Magnusson R, Ding Y, Lee K J, Priambodo P S and Wawro D 2005 *International Society for Optics and Photonics* (Boston MA 23 October 2005 60080U-160080U-10)
[4] Cheben P, Janz S, Xu D X, Lamontagne B, Delage A and Tanev S 2006 *IEEE Photon. Technol. Lett.* **18** 13
[5] Mateus C F R, Huang M C Y, Deng Y F, Neureuther A R and Chang-Hasnain C J 2004 *IEEE Photon. Technol. Lett.* **16** 518
[6] Zhou Y, Huang M C Y, Chase C, Karagodsky V, Moewe M, Pesala B, Sedgwick F G and ChangHasnain C J 2009 *IEEE J. Sel. Top. Quantum Electron.* **15** 1485
[7] Fano U 1961 *Phys. Rev.* **124** 1866
[8] Zhou Y, Moewe M, Kern J, Huang M C Y and ChangHasnain C J 2008 *Opt. Express* **16** 17282
[9] Karagodsky V, Chase C and Chang-Hasnain C J 2011 *Opt. Lett.* **36** 1704
[10] Ahmed A, Liscidini M and Gordon R 2010 *IEEE Photon. J.* **2** 884
[11] Wu T T, Wu S H, Lu T C and Wang S C 2013 *Appl. Phys. Lett.* **102** 081111
[12] Moharam M G, Pommet D A, Grann E B and Gaylord T K 1995 *J. Opt. Soc. Am.* A **12** 1077
[13] Moharam M G, Grann E B, Pommet D A and Gaylord T K 1995 *J. Opt. Soc. Am.* A **12** 1068
[14] Taflove A and Hagness S C 2005 *Computational Electrodynamics: The Finite-Difference Time-Domain Method* 3rd edn (Massachusetts: Artech House)
[15] Fan S, Suh W and Joannopoulos J D 2003 *J. Opt. Soc. Am.* A **20** 569
[16] Cao L Y, Fan P Y and Brongersma M L 2011 *Nano Lett.* **11** 1463
[17] Huang L J, Yu Y L and Cao L Y 2013 *Nano Lett.* **13** 3559
[18] Komarevskiy N, Shklover V, Braginsky L and Hafner C 2013 *Prog. Eletromagn. Res.* **139** 799
[19] Yu Y L and Cao L Y 2012 *Opt. Express* **20** 13847
[20] Haus H A 1984 *Wave and Fields in Optoelectronics* (New Jersey: Prentice-Hall)
[21] Rytov S M 1956 *Sov. Phys. JETP* **2** 466
[22] Wolf M and Born E 1999 *Principles of Optics: Electromagnetic Theory of Propagation, Interference and Diffraction of Light* 7th (expanded) edn (Cambridge: Cambridge University Press)
[23] Liu W X, Li Y H, Jiang H T, Lai Z Q and Chen H 2013 *Opt. Lett.* **38** 163