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Propagation of electromagnetic radiation through a one-dimensional superlattice doped with impurity plasma layers

Vladimir Rumyantsev[a,b], Stanislav Fedorov[b], Kostyantyn Gumennyk[b,*], Marina Sychanova[b]

[a] Mediterranean Institute of Fundamental Physics, Marino, Rome 00047, Italy
[b] Galkin Institute for Physics and Engineering, Donetsk 83114, Ukraine

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ABSTRACT

The virtual crystal approximation is employed to carry out a numerical modeling of a nonideal one-dimensional Si-based photonic crystal comprised of topologically ordered sets of layers with randomly included doping plasma layers. The constructed model proves efficient for evaluation of the photonic band gap as a function of plasma layer concentration. The presence of defect layers is shown to significantly alter the photonic spectrum of the superstructure. Calculations show that an appropriate choice of dopant concentration is capable of reducing the band gap to zero, thus turning the lattice into a frequency filter.

1. Introduction

Until very recently the propagation of electromagnetic waves in layered crystalline media has been drawing an unabating attention [1–3]. Tolmachov et al. gave a survey of studies devoted to silicon- and liquid crystal-based photonic structures [4]. Zhang et al. used the plane wave expansion method to investigate the properties of photonic band gaps in three-dimensional plasma photonic crystals composed of isotropic dielectric and unmagnetized plasma with diamond lattices [5,6]. An interest for these objects is on one hand explained by their significance for electronics, and on the other hand is due to the progress in methods of the growth of ultrathin films and periodic structures with controllable characteristics.

There are numerous theoretical and experimental studies devoted to exciton-like excitations in ideal dielectric superlattices. A general theory of optical waves in anisotropic crystals, including those, formed of macroscopic layers, is discussed in a well-known book by Yariv and Yeh [7]. Further advance of the theory of layered structures requires the adoption of more complex models such as that of a superlattice with randomly included impurity layers. An understanding of the effect of such admixtures on optical properties of the corresponding systems is indispensable for the effective manufacturing of layered materials with desirable characteristics.

The methods of calculation of polaritonic excitation spectra are quite similar to those used in the cases of electronic, phononic and other types of quasiparticle excitations. In the present paper we utilize the virtual crystal approximation (VCA) [8,9], which is based on the configurational averaging technique to study polaritonic excitations in a *macroscopically* inhomogeneous medium. Until now this method has been applied for *microscopic* calculations of quasiparticle excitation spectra in disordered systems. The main idea of the VCA consists in replacement of configurationally dependent Hamiltonian parameters by their configurationally averaged values.

An efficient description of transformation of polaritonic spectra in simple superlattices caused by doping layers is essential for the study of imperfect layered structures. Evaluation of polaritonic spectra and of related quantities (such as the density of states of elementary excitation as well as various characteristics of normal electromagnetic waves etc.) in less simple systems usually requires the use of more complex methods. Such can be the method of coherent potential [11] or the averaged T-matrix method [10,12].

In what follows we model a superlattice as a set of macroscopically homogeneous layers with randomly included foreign

* Corresponding author. Tel.: +380 958202210.
E-mail address: kgumennyk@gmail.com (K. Gumennyk).

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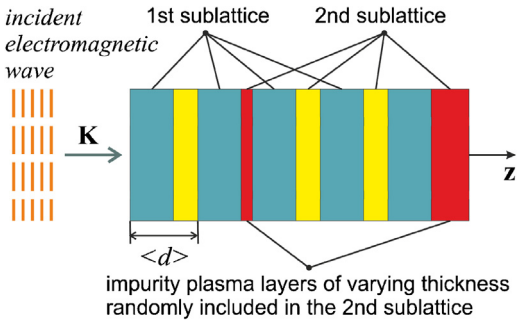

Fig. 1. A two-sublattice superstructure with randomly included (in the 2nd sublattice) impurity layers.

(with respect to an ideal structure) layers of variable thicknesses (Fig. 1). Configuration-dependent material tensors of the imperfect superlattice are expressed through the appropriate random quantities. Configurational averaging "restores" the translational symmetry of the considered structure and permits to obtain a system of equations, which define the normal modes of electromagnetic waves, propagating through the resulting one-dimensional "periodic" medium.

2. The model

Dielectric $\hat{\varepsilon}(\mathbf{r})$ and magnetic $\hat{\mu}(\mathbf{r})$ permeabilities, which determine optical characteristics of a periodic medium are subject to periodic boundary conditions:

$$\hat{\varepsilon}(x,y,z)=\hat{\varepsilon}(x,y,z+d),\quad \hat{\mu}(x,y,z)=\hat{\mu}(x,y,z+d),$$

where $d=\sum_{j=1}^{\sigma}a_j$ is the superlattice period, σ is the number of layers per one elementary cell, a_j are the thicknesses of layers, which form a one-dimensional chain of elements oriented along the z-axis. Material tensors $\hat{\varepsilon}$ and $\hat{\mu}$ of a crystalline superlattice with an arbitrary number of layers σ have the following coordinate representation [13]:

$$\begin{pmatrix}\hat{\varepsilon}(z)\\ \hat{\mu}(z)\end{pmatrix}=\sum_{n,\alpha}\begin{pmatrix}\hat{\varepsilon}_{n\alpha}\\ \hat{\mu}_{n\alpha}\end{pmatrix}\left\{\theta\left[z-(n-1)d-\left(\sum_{j=1}^{\alpha}a_{nj}-a_{n\alpha}\right)\right]-\theta\left[z-(n-1)d-\sum_{j=1}^{\alpha}a_{nj}\right]\right\}. \quad (1)$$

Here $\theta(z)$ is the Heaviside step function, index $n=\pm1,\pm2,\ldots$ numerates one-dimensional crystal cells, whereas $\alpha=1,2,\ldots,\sigma$ numerates elements in a cell. Within our model the configurationally dependent tensors $\hat{\varepsilon}_{n\alpha}$, $\hat{\mu}_{n\alpha}$, $a_{n\alpha}$ are expressed through the random quantities $\eta_{n\alpha}^{\nu}$, where $\eta_{n\alpha}^{\nu}=1$ if the $\nu(\alpha)$th type of layer occupies the $(n\alpha)$th site of the one-dimensional crystalline lattice, and $\eta_{n\alpha}^{\nu}=0$ otherwise:

$$\begin{pmatrix}\hat{\varepsilon}_{n\alpha}\\ \hat{\mu}_{n\alpha}\end{pmatrix}=\sum_{\nu(\alpha)}\begin{pmatrix}\hat{\varepsilon}_{\alpha}^{\nu(\alpha)}\\ \hat{\mu}_{\alpha}^{\nu(\alpha)}\end{pmatrix}\eta_{n\alpha}^{\nu(\alpha)},\ a_{n\alpha}=\sum_{\nu(\alpha)}a_{\alpha}^{\nu(\alpha)}\eta_{n\alpha}^{\nu(\alpha)}. \quad (2)$$

By analogy with the quasi-particle approach the VCA is used here to calculate polaritonic spectrum of the imperfect superlattice using the following replacements: $\hat{\varepsilon}\to\langle\hat{\varepsilon}\rangle$, $\hat{\mu}\to\langle\hat{\mu}\rangle$ (and $d\to\langle d\rangle$, $a_{n\alpha}\to\langle a_{n\alpha}\rangle$ for variable thickness of layers). Angular parentheses designate the procedure of configuration averaging. Eq. (2) yields

$$\begin{pmatrix}\langle\hat{\varepsilon}_{n\alpha}\rangle\\ \langle\hat{\mu}_{n\alpha}\rangle\end{pmatrix}=\sum_{\alpha,\nu(\alpha)}\begin{pmatrix}\hat{\varepsilon}_{\alpha}^{\nu(\alpha)}\\ \hat{\mu}_{\alpha}^{\nu(\alpha)}\end{pmatrix}C_{\alpha}^{\nu(\alpha)},\quad \langle a_{n\alpha}\rangle=\sum_{\upsilon(\alpha)=1}^{r(\alpha)}a_{\alpha}^{\upsilon(\alpha)}C_{\alpha}^{\upsilon(\alpha)} \quad (3)$$

where $C_{\alpha}^{\nu(\alpha)}$ is concentration of the $\nu(\alpha)$th sort of impurity layers contained in the αth sublattice. There must hold an obvious relation $\sum_{\nu(\alpha)}C_{\alpha}^{\nu(\alpha)}=1$. In the framework of the virtual crystal approximation the problem of finding of the main quantities of interest (such as the spectrum, the band gap etc.) as well as the problem of finding of polaritonic characteristics is reduced to an analogous problem for an ideal multilayer material with the averaged permeabilities $\langle\hat{\varepsilon}\rangle$ and $\langle\hat{\mu}\rangle$, widths of layers $a_{\alpha}\left\{C_{\alpha}^{\nu(\alpha)}\right\}$ and period $d\left\{C_{\alpha}^{\nu(\alpha)}\right\}$. From Eq. (1) it follows that Fourier-amplitudes $\hat{\varepsilon}_l$, $\hat{\mu}_l$ and the averaged dielectric $\langle\hat{\varepsilon}_{n\alpha}\rangle$ and magnetic $\langle\hat{\mu}_{n\alpha}\rangle$ permeabilities of layers (3) are related as

$$\begin{pmatrix}\hat{\varepsilon}_l\\ \hat{\mu}_l\end{pmatrix}=-\frac{i}{2\pi l}\sum_{\alpha}\begin{pmatrix}\langle\hat{\varepsilon}_{n\alpha}\rangle\\ \langle\hat{\mu}_{n\alpha}\rangle\end{pmatrix}\times\left\{\exp\left(i\frac{2\pi}{d\left\{C_{\alpha}^{\nu(\alpha)}\right\}}l\sum_{j=1}^{\alpha}a_j\left\{C_{\alpha}^{\nu(\alpha)}\right\}\right)-\exp\left[i\frac{2\pi}{d\left\{C_{\alpha}^{\nu(\alpha)}\right\}}l\left(\sum_{j=1}^{\alpha}a_j\left\{C_{\alpha}^{\nu(\alpha)}\right\}-a_{\alpha}\left\{C_{\alpha}^{\nu(\alpha)}\right\}\right)\right]\right\} \quad (4)$$

Since configurational averaging "restores" the translation symmetry of the one-dimensional imperfect superlattice we can write the Maxwell equations for amplitudes $\mathbf{E}(\mathbf{r},\omega)$, $\mathbf{H}(\mathbf{r},\omega)$ of the harmonic time dependencies of the electric and magnetic fields. According to Floquet theorem the Fourier-amplitudes $\mathbf{f}_{K,p}^{(E,H)}$ of electric and magnetic field strengths satisfy the relation:

$$\left[\boldsymbol{\beta}+\left(K+p\frac{2\pi}{d\left\{C_{\alpha}^{\nu(\alpha)}\right\}}\right)\mathbf{e}_z\right]\times\begin{pmatrix}\mathbf{f}_{K,p}^{(H)}\\ \mathbf{f}_{K,p}^{(E)}\end{pmatrix}=\frac{\omega}{c}\begin{bmatrix}-\sum_l\hat{\varepsilon}_l\cdot\mathbf{f}_{K,p-l}^{(E)}\\ \sum_l\hat{\mu}_l\cdot\mathbf{f}_{K,p-l}^{(H)}\end{bmatrix}, \quad (5)$$

where $\boldsymbol{\beta}$ is an arbitrary planar (lying in XOY plane) wave vector, $\mathbf{e}_z$ is a unit vector directed along the z-axis, $\mathbf{K}=(0,0,K)$ is the Bloch vector. System (5) defines the normal modes of electromagnetic waves, propagating through the considered "periodic" medium. For simplicity, we shall restrict our study to the case of light propagation along the z-axis ($\boldsymbol{\beta}=0$) in a nonmagnetic lattice ($\hat{\mu}=\hat{I}$ being a unit matrix) with uniaxial liquid–crystal layers $\varepsilon_{ij}=\varepsilon_{xx}\delta_{xi}\delta_{jx}+\varepsilon_{yy}\delta_{yi}\delta_{jy}+\varepsilon_{zz}\delta_{zi}\delta_{jz}$. It is obvious, that for $\mathbf{K}\|z$ the zz-components of tensor $\hat{\varepsilon}$ do not appear in the resulting formulas and $\varepsilon_{xx}=\varepsilon_{yy}\equiv\varepsilon$. Furthermore, similarly to Ref. [6] we shall assume that the value of K is close to the one defined by Bragg's condition: $\left|K-\left(2\pi/d\right)\right|\approx K$, $c^2K^2\approx\omega^2\varepsilon_0$. Under these circumstances, the only essential Fourier-components $\mathbf{f}_{K,p}^{(E,H)}$ of electromagnetic plane waves are the ones with $p=0$ and -1. Retaining these components in Eq. (5) we arrive at the following equation:

$$\begin{bmatrix}K^2-\frac{\omega^2}{c^2}\varepsilon^{(0)} & -\frac{\omega^2\varepsilon^{(1)}}{c^2}\\ -\frac{\omega^2\varepsilon^{(-1)}}{c^2} & \left(K-\frac{2\pi}{d\left\{C_{\alpha}^{\nu(\alpha)}\right\}}\right)^2-\frac{\omega^2}{c^2}\varepsilon^{(0)}\end{bmatrix}\begin{pmatrix}f_{K,0}^{(E)}\\ f_{K,-1}^{(E)}\end{pmatrix}=0, \quad (6)$$

where $\varepsilon_{l=0}\equiv\varepsilon^{(0)}$, $\varepsilon_{l=\pm1}\equiv\varepsilon^{(\pm1)}$. The dispersion relations $\omega_{\pm}=\omega(K)$ are obtained from the system (6) by setting its determinant equal to zero. The two roots of the resulting equation $\omega_{\pm}$ define the spectral band boundaries. For frequencies falling within the band gap $\omega_{-}(K)<\omega<\omega_{+}(K)$ the said roots are complex and therefore