Tamm Polaritons and Cavity Modes in the FIR Range

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ABSTRACT
Tamm polaritons (TPs) are formed at the interface between two semi-infinite periodic dielectric structures (Bragg mirrors) or other reflectors. Contrary to usual surface polaritons, TPs exist inside the "light cone", even though their amplitude also decreases exponentially with the distance from the interface as it is characteristic of evanescent waves. They couple to elementary excitations in the materials or structures that form the interface, such as metal plasmons or semiconductor excitons. Here we discuss the formation of TPs in the far-infrared (FIR) spectral range, in the optical-phonon reststrahlen band of a polar semiconductor such as GaAs, with a Bragg reflector (BR) as the second mirror. Their dispersion relation and the frequency window for the TP existence are discussed for a GaAs-BR interface and also structures containing a gap between the two reflectors.
Keywords: Bragg reflector, semiconductor, phonon, optical Tamm state.

1. INTRODUCTION

The possibility of existence of interface electromagnetic (EM) waves at the interface between two reflecting media, analogous to electronic Tamm states arising at the surface of a crystal because of the broken translational symmetry [1], has been predicted theoretically for two semi-infinite periodic dielectric structures (that can be named superlattices or 1D photonic crystals or simply Bragg reflectors, BRs) [2] and later for a gold slab combined with a dielectric BR [3]. Such waves were called Tamm polaritons or optical Tamm states (OTSs). Contrary to the electronic Tamm states, OTSs cannot occur at a free surface but only at the interface between two photonic structures having overlapping photonic band gaps (or stop bands). The existence of Tamm plasmon-polaritons has been demonstrated experimentally in Refs. [4, 5] for GaAs/AlGaAs superlattices covered with a gold layer. More recently, coupling of OTSs to excitons in a 2D semiconductor layer has been demonstrated [6], leading to the formation of room-temperature exciton-polaritons where the excitons are localized in an atomically thin layer while the EM field is confined (at a much larger scale) within a planar microcavity [7]. While the formation of plasmon-polaritons, with an exponentially decaying amplitude inside the metal is due to the negative dielectric constant of the metal below its plasma frequency, in the latter case the exciton has no role in the formation of the OTS but just couples to it. The metal film was used as adjustable means for making a microcavity (sometimes called Tamm microcavity) [8].

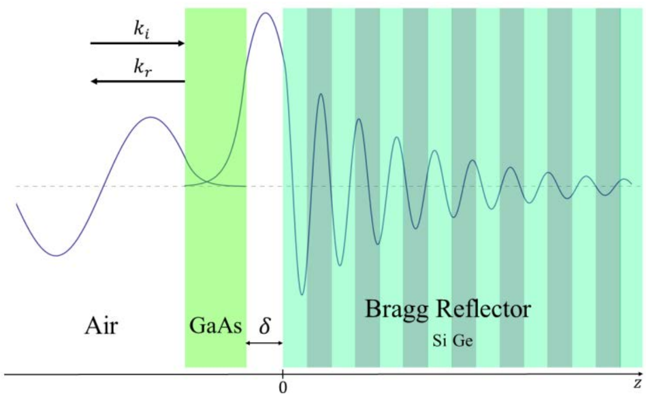

Figure 1. Schematics of the studied heterostructure and qualitative profiles of the electric field amplitude corresponding to OTS and external EM wave in air used for probing this confined state. GaAs layer and BR are separated by an air gap of thickness δ (a microcavity).

The purpose here is to extend these ideas to a different (namely FIR) spectral range and to find states at the interface between a polar semiconductor (such as GaAs) and a Bragg reflector suitable for the far-infrared (FIR) range. Within the frequency range between the transverse (ω_{TO}) and longitudinal (ω_{LO}) optical phonon frequencies (known as reststrahlen band), the real part of the dielectric function of the semiconductor is negative [9]. Therefore, the semiconductor acts as a mirror in this frequency range, similar to a metal but it is less lossy because the imaginary part peaks at ω_{TO} and the width of this peak is just few cm^{-1} for a good crystal, while the width of the reststrahlen band is typically a few tens of cm^{-1}. As known, multilayer structures containing polar semiconductors support evanescent waves named surface phonon-polaritons, which occur in their reststrahlen band [10, 11]. Such polaritons are characterized by an imaginary wavevector component in the direction perpendicular to the surface (to be denoted as z direction), i.e. their dispersion curve lies outside of the light cone. In contrast, OTSs have a real z-component of the wavevector. The EM field confinement in the multilayer structure (used as the second mirror) is due to a photonic stop band of the Bragg reflector (see Fig. 1). The materials chosen for our model calculations are GaAs, a semiconductor with $\omega_{TO} = 268\ \text{cm}^{-1}$ and $\omega_{LO} = 292\ \text{cm}^{-1}$ [9], and silicon and germanium for the BR, two compatible materials which are non-absorbing in the relevant frequency range. The Tamm polaritons are expected in the frequency range where the BR stop band and the reststrahlen band of GaAs overlap. We shall explore their dispersion relation considering both the "pure" Tamm state ($\delta = 0$ in Fig. 1) and cavity modes ($\delta \neq 0$).

2. TRANSFER MATRIX METHOD

We begin by presenting the transfer matrix formalism, which is very convenient for multilayer planar structures studied in this work. Let us consider a superlattice consisting in a periodic structure of stacked alternating layers of Si and Ge of equal thickness, with a period $2d$. Their dielectric constants are denoted ϵ_A and ϵ_B. For oblique incidence of a wave coming from $z < 0$ (with the angle of incidence θ) we have to take into account the electric and magnetic fields perpendicular and parallel to the surface, corresponding to s-polarization (or TE waves) and p-polarization (or TM waves). An arbitrarily polarized field plane wave can be written as the superposition of two orthogonally polarized plane waves:

$$\boldsymbol{E} = \boldsymbol{E}^{(s)} + \boldsymbol{E}^{(p)}; \quad \boldsymbol{H} = \boldsymbol{H}^{(s)} + \boldsymbol{H}^{(p)}, \tag{1}$$

where the electric field components of the two waves are perpendicular and parallel to the incidence plane, respectively. Let us confine ourselves by considering only p-polarization here. Our purpose is to calculate the reflection and transmission Fresnel coefficients, $\hat{r}^{(p)}$and $\hat{t}^{(p)}$, defined as [12]:

$$\boldsymbol{H}_r^{(p)} = \hat{r}^{(p)} \cdot \boldsymbol{H}_i^{(p)}; \quad \boldsymbol{H}_t^{(p)} = \hat{t}^{(p)} \cdot \boldsymbol{H}_i^{(p)}, \tag{2}$$

with the subscripts i, r and t referring to the incident, reflected and transmitted waves. For p-polarization the magnetic field is parallel to the surface (to be denoted as y direction),

$$\boldsymbol{H}_i^{(p)} = \hat{y}\, H_i\, e^{i(\boldsymbol{k}_i \cdot \boldsymbol{r} - \omega t)}, \quad \boldsymbol{H}_r^{(p)} = \hat{y}\, H_r\, e^{i(\boldsymbol{k}_i \cdot \boldsymbol{r} - \omega t)}, \quad \boldsymbol{H}_t^{(p)} = \hat{y}\, H_t\, e^{i(\boldsymbol{k}_i \cdot \boldsymbol{r} - \omega t)}. \tag{3}$$

The transfer matrix for one Si/Ge bilayer is determined by using the solution of the Maxwell equations within each layer in the form of standing waves and applying the continuity conditions at the boundaries:

$$\begin{pmatrix} H_1(\boldsymbol{r},t) \\ E_{1x}(\boldsymbol{r},t) \end{pmatrix}_{z=0^-} = \begin{pmatrix} H_A(\boldsymbol{r},t) \\ E_{Ax}(\boldsymbol{r},t) \end{pmatrix}_{z=0^+}, \tag{4}$$

where the index y in the magnetic field component was skipped for clarity, the index 1 refers to the fields in air at $z < 0$,

$$\begin{pmatrix} H_A(\boldsymbol{r},t) \\ E_{Ax}(\boldsymbol{r},t) \end{pmatrix}_{z=0^+} = \hat{T}_A^{-1} \cdot \begin{pmatrix} H_A(\boldsymbol{r},t) \\ E_{Ax}(\boldsymbol{r},t) \end{pmatrix}_{z=d^-} = \hat{T}_A^{-1} \cdot \begin{pmatrix} H_B(\boldsymbol{r},t) \\ E_{Bx}(\boldsymbol{r},t) \end{pmatrix}_{z=d^+}, \tag{5}$$

and

$$\begin{pmatrix} H_B(\boldsymbol{r},t) \\ E_{Bx}(\boldsymbol{r},t) \end{pmatrix}_{z=d^+} = \hat{T}_B^{-1} \cdot \begin{pmatrix} H_B(\boldsymbol{r},t) \\ E_{Bx}(\boldsymbol{r},t) \end{pmatrix}_{z=2d^-}. \tag{6}$$

where the matrices $\hat{T}_A$ and $\hat{T}_B$ are given by:

$$\hat{T}_{A,B}^{-1} = \begin{pmatrix} \cos(k_{A,B}d) & i\dfrac{\omega\epsilon_{A,B}}{ck_{A,B}}\sin(k_{A,B}d) \\ i\dfrac{ck_{A,B}}{\omega\epsilon_{A,B}}\sin(k_{A,B}d) & \cos(k_{A,B}d) \end{pmatrix} \tag{7}$$

with

$$k_{A,B} = \sqrt{\epsilon_{A,B}^2 \left(\frac{\omega}{c}\right)^2 - q^2} \tag{8}$$

where $q = \omega/c \sin\theta$ is the in-plane wavevector. Thus,

$$\begin{pmatrix} H_1(\boldsymbol{r},t) \\ E_{1x}(\boldsymbol{r},t) \end{pmatrix}_{z=0^-} = \hat{T}_A^{-1} \cdot \hat{T}_B^{-1} \cdot \begin{pmatrix} H_B(\boldsymbol{r},t) \\ E_{Bx}(\boldsymbol{r},t) \end{pmatrix}_{z=2d^-}. \tag{9}$$

Consequently, for an N-period structure, we have:

$$\begin{pmatrix} H_1(\boldsymbol{r},t) \\ E_{1x}(\boldsymbol{r},t) \end{pmatrix}_{z=0^-} = (\hat{T}_A^{-1} \cdot \hat{T}_B^{-1})^N \cdot \begin{pmatrix} H_B(\boldsymbol{r},t) \\ E_{Bx}(\boldsymbol{r},t) \end{pmatrix}_{z=2Nd^-}. \tag{10}$$

Connecting to the fields in the medium on the right of the superlattice (index 3) yields:

$$\begin{pmatrix} H_1(\boldsymbol{r},t) \\ E_{1x}(\boldsymbol{r},t) \end{pmatrix}_{z=0^-} = (\hat{T}_A^{-1}\cdot\hat{T}_B^{-1})^N \cdot \begin{pmatrix} H_B(\boldsymbol{r},t) \\ E_{Bx}(\boldsymbol{r},t) \end{pmatrix}_{z=2Nd^-} = (\hat{T}_A^{-1}\cdot\hat{T}_B^{-1})^N \cdot \begin{pmatrix} H_3(\boldsymbol{r},t) \\ E_{3x}(\boldsymbol{r},t) \end{pmatrix}_{z=2Nd^+}. \quad (11)$$

Expressing the fields in the media 1 and 3 in terms of the incident, reflected and transmitted waves, we obtain:

$$\begin{pmatrix} 1+\hat{r}^{(p)} \\ \frac{ck_{1z}}{\epsilon_1\omega}(1-\hat{r}^{(p)}) \end{pmatrix} = \hat{T}_N^{-1}\cdot\begin{pmatrix} \hat{t}^{(p)} \\ -\frac{ck_{3z}}{\epsilon_3\omega}\hat{t}^{(p)} \end{pmatrix}, \quad (12)$$

where $\hat{T}_N^{-1}$ is the inverse transfer matrix of the whole structure, $\hat{T}_N^{-1} = (\hat{T}_A^{-1}\cdot\hat{T}_B^{-1})^N$. From Eq. (12) one readily obtains the Fresnel coefficients of the structure.

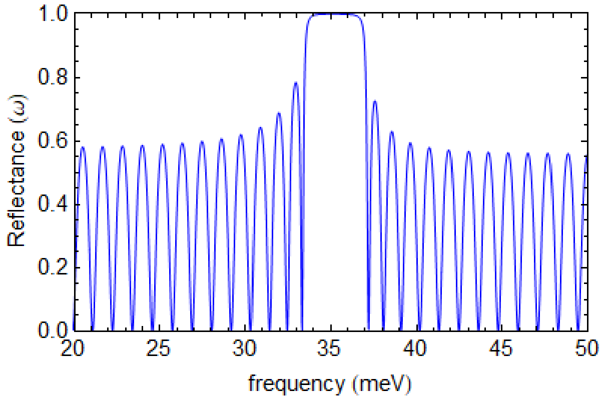

Figure 2. Reflectivity spectrum of a Si/Ge BR with $d = 2.4$ *μm.*

The reflectivity $\left(R = \left|\hat{r}_1^{(p)}\right|\right)$ spectrum calculated for N =100 is shown in Fig. 2. The period of the superlattice was chosen in such a way that the stop band (the frequency range where the reflectivity is close to unity) matches the reststrahlen band of GaAs. The position of the band shows little dependence upon the angle of incidence. On the other hand, it strongly depends on the thickness of the layers, on the period of the superlattice and on the contrast of the refractive index between materials A and B. If the contrast of the refractive index is not too small, several tens of periods already yield an almost perfect stop band.

3. OPTICAL TAMM STATES: DISPERSION RELATION AND PROBING

Now we shall derive the dispersion relation for OTS eigenmodes of the structure shown in Fig. 1. Let $\hat{T}_1$ and $\hat{T}_2$ be the transfer matrices of the GaAs layer and the Bragg reflector, respectively. We consider that there is no incident wave but there are only "transmitted" (i.e. outgoing) waves at both sides of the whole structure. By analogy with Eqs. (11) and (12) we can write for the fields at $z = 0$:

$$\hat{T}_2\cdot\begin{pmatrix} \hat{t}_2^{(p)} \\ \hat{t}_2^{(p)}\frac{ck}{\omega} \end{pmatrix} = \hat{T}_\delta^{-1}\cdot\hat{T}_1^{-1}\cdot\begin{pmatrix} \hat{t}_1^{(p)} \\ -\hat{t}_1^{(p)}\frac{ck}{\omega} \end{pmatrix}. \quad (13)$$

where $k = (\omega/c)\cos\theta$ and the subscripts 1 and 2 here refer, respectively, to the media on the left and on the right of the heterostructure. By setting $\hat{t}_1^{(p)} = A\hat{t}_2^{(p)}$ where A is a complex number, we obtain:

$$\hat{T}_1\cdot\hat{T}_\delta\cdot\hat{T}_2\cdot\begin{pmatrix} 1 \\ \frac{ck}{\omega} \end{pmatrix} = A\begin{pmatrix} 1 \\ -\frac{ck}{\omega} \end{pmatrix}. \quad (14)$$

Here $\hat{T}_\delta$ is the transfer matrix of the δ-layer, also of the form (7). By eliminating A with the use of two lines of Eq. (14) one obtains an explicit dispersion relation, $\omega(q)$, of the OTSs. It can be cast in another form by using the relation (12) between the Fresnel coefficients, which reads

$$\hat{r}_1^{(p)}\hat{r}_2^{(p)}e^{2ik\delta} = 1. \quad (15)$$

Assuming that the mirrors are perfect, $\left|\hat{r}_1^{(p)}\right|\left|\hat{r}_2^{(p)}\right|$=1, Eq. (15) is equivalent to the following phase matching condition:

$$\Delta\varphi \equiv \varphi_1 + \varphi_2 + 2k\delta = 2\pi m, \quad (16)$$

where $\varphi_{1,2} = \arg(\hat{r}_{1,2}^{(p)})$ and m is and integer. It determines the Tamm modes in the structure.

The dispersion relation calculated by substituting different angles θ into Eq. (16) is approximately parabolic with ω increasing with q for $\delta = 0$, see Fig. 3c. For $\delta \neq 0$ (Tamm microcavity) the dispersion curves shift downwards within the reststrahlen band and their shape deviates from parabolic.

OTSs can be probed by measuring the reflectivity spectrum of the whole structure. Coupling of the incident (propagating) wave to the Tamm mode occurs owing to the (exponentially small) overlap between two decaying waves, one originated by the incident EM wave and the other corresponding to the Tamm state as depicted in Fig. 1. Even though the GaAs slab is not a perfect mirror for the frequencies close to ω_{LO} (since the real part of the dielectric function is only slightly negative and $|\hat{r}_{GaAs}| < 1$), the phase matching condition (16) is a fairly good indication of the OTS as illustrated in Fig. 3. The reflectivity, calculated through the Fresnel coefficient of the whole structure, which is obtained from Eq. (12) with the "global" transfer matrix, $\hat{T}_G = \hat{T}_1 \cdot \hat{T}_\delta \cdot \hat{T}_2$, shows a sharp dip at a frequency close to that corresponding to $\Delta\varphi = 0$ (see Figs. 3a and 3b). The coupling affects the Tamm state's frequency, so the exact position of the spectral dip slightly deviates from the proper Tamm mode and depends on the thickness of the GaAs layer.

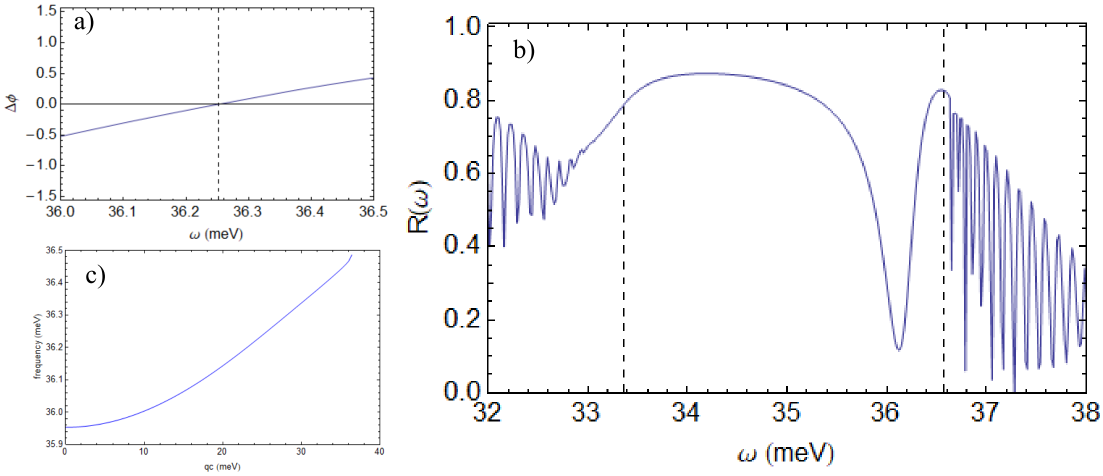

Figure 3: (a) Phase matching condition determining the OTS frequency and (b) the corresponding reflection spectrum; dispersion relation of the OTS (frequency vs in-plane wavevector) for $\delta = 0$*. In the phase matching equation the GaAs phonon damping was set equal to zero. Parameters:* $d = 2.4\ \mu m$, $d_{GaAs} = 5\ \mu m$.

To conclude, we have shown that Tamm polaritons can be supported by structures where EM field confinement is due to polar optical phonons and takes place in the reststrahlen band of the semiconductor. For $\delta = 0$ their dispersion is approximately parabolic with a positive effective mass, similar to that obtained in Ref. [3] for a gold-GaAs/AlAs superlattice heterostructure. While Tamm states in the near-IR spectral range have been observed experimentally [4, 5], the performed calculations show that one can also search for OTSs in the FIR region using GaAs (or other polar semiconductor) as a phononic mirror.

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REFERENCES

[1] I.E. Tamm, *Phys. Z. (Soviet Union)*, vol. 1, p. 733 (1932) .
[2] A.V. Kavokin, *Phys. Rev. B*, vol. 72, p. 233102 (2005).
[3] M. Kaliteevski *et al.*, *Phys. Rev. B*, vol. 76, p. 165415 (2007).
[4] M.E. Sasin *et al.*, *Appl. Phys. Lett.*, vol. 92, p. 251112 (2008).
[5] M.E. Sasin *et al.*, *Superlattices and Microstructures*, vol. 47, p. 44 (2010).
[6] N. Lundt *et al.*, *Nature Communications*, vol. 6, p. 13328 (2016).
[7] M.I. Vasilevskiy *et al.*: *Phys. Rev. B*, vol. 92, p. 245435 (2015).
[8] K. Sebald *et al.*, *Appl. Phys. Lett.*, vol. 107, p. 062101 (2015).
[9] P.Y. Yu and M. Cardona, *Fundamentals of Semiconductors*, Springer-Verlag, Berlin, 1996.
[10] E.A. Vinogradov, *Physics - Uspekhi*, vol. 45, p. 1213 (2002).
[11] M.F. Cerqueira *et al.*, *J. Phys. D: Applied Physics*, vol. 50, p. 365103 (2017) .
[12] L. Novotny and B. Hecht, *Principles of Nanooptics*, Cambridge University Press, Cambridge, UK, 2012.