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Surface and interface phonon-polaritons in freestanding quantum well wire systems of polar ternary mixed crystals



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HIGHLIGHTS

- We study surface and interface phonon-polaritons in freestanding QWW systems.
- Polariton modes located in the three forbidden bands of bulk phonon-polaritons.
- Polariton properties depend on the geometric structure and composition of the TMC.
- One or two mode behaviors of surface and interface phonon-polaritons are seen.

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ABSTRACT

The surface and interface phonon-polaritons in freestanding rectangular quantum well wire systems consisting of polar ternary mixed crystals are investigated in the modified random-element-iso-displacement model and the Born-Huang approximation, based on the Maxwell's equations with the boundary conditions. The numerical results of the surface and interface phonon-polariton frequencies as functions of the wave-vector, geometric structure, and the composition of the ternary mixed crystals in GaAs/Al_xGa_{1-x}As and Zn_xCd_{1-x}Se/ZnSe quantum well wire systems are obtained and discussed. It is shown that there are 10 and 8 branches of surface and interface phonon-polaritons in the two quantum well wire systems respectively. The effects of the "two-mode" and "one-mode" behaviors of the ternary mixed crystals on the surface and interface phonon-polariton modes are shown in the dispersion curves.

1. Introduction

The investigation of optical and electronic properties in semiconductor nanostructures, such as quantum wells, quantum well wires, and quantum dots, have been a subject of great interest in recent years [1–3]. Surface and interface phonon-polaritons, which are mixed electromagnetic modes resulting from the coupling of photons and infrared active phonons localized near the surface or interface of different media, have attracted considerable interest for decades. It is generally known that the knowledge of surface and interface phonon-polaritons is significant to understand the characteristic of semiconductor nanosystems. The surface and interface phonon-polaritons in quasi-two-dimensional systems have been extensively investigated both in experiments and theories [4–13].

Surface and interface phonon-polaritons have been observed in some layered systems by using methods of Raman scattering and attenuated total reflection (ATR) experimentally. Marschall and Fischer were the first who observed a surface phonon-polariton mode in a semi-infinite GaP crystal by using ATR technique [4]. Evans, Ushioda and McMuller have observed the Raman scattering from surface phonon-polaritons in a thin film of GaAs on a sapphire substrate [5]. Later, Nakayama and his collaborators studied the interface phonon-polaritons in a GaAs/AlAs heterostructure system by means of Raman scattering [6]. Recently, Lee et al. have investigated the surface phonon-polaritons of hexagonal sapphire crystals with non-polar and semi-polar crystallographic planes by the polarized infrared ATR measurements [7].

The classical electromagnetic theory of surface and interface phonon-polaritons in a film has been first presented by Mills and Maradudin [8]. Their results showed that the surface and interface phonon-polaritons lie between longitudinal optical (LO) and transverse optical (TO) phonon frequencies of polar crystal, where the dielectric function is negative. Later, surface and interface phonon-polaritons in heterostructures [9], bilayer systems [10], quantum wells [11], superlattices [12], and quantum wires [13] have been

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investigated by using the method of classical electromagnetic theory.

However, to the best of our knowledge, the surface and interface phonon-polaritons in freestanding quantum well wires (QWWs) of ternary mixed crystals (TMCs) have rarely been investigated. It is well known that TMC material possess great applied potentials in light emitting diodes, laser diodes, and other optoelectronic devices due to their excellent properties [14–16]. The surface and interface phonon-polaritons in low-dimensional systems of TMCs may reveal many distinct features than that in the systems of binary crystals owing to their complicated properties of lattice vibrations [17,18]. Therefore, a detailed theoretical investigation of surface and interface phonon-polaritons in free-standing QWWs is necessary.

In this paper we study theoretically the surface and interface phonon-polaritons in freestanding rectangular QWW systems composed of TMCs, within the framework of modified random-element-isodisplacement (MREI) model [18] and the Born–Huang approximation [19], based on the Maxwell's equations with the boundary condition. The frequencies of the surface and interface phonon-polaritons are calculated and the numerical results for several III–V and II–VI systems are obtained and discussed.

2. Formulation

In this paper, we consider a freestanding QWW system composed of polar TMC material of infinite in the z direction with the well material "1" (localized in the region of $|x| \le d_1$ and $|y| \le d_1$) surrounded by barrier material "2" (in the region of $|x| \le d_2$ and $|y| \le d_2$) in the x and y directions, respectively, as shown in Fig. 1. Surface and interface phonon-polaritons are traveling along the z direction with the wave vector k_z , and the electric field E lies in the x-z (y-z) plane, and the magnetic field E is along the y-(x-) axis.

The electric field can be taken as

$$\vec{E}(\vec{r}) = \vec{E}(x, y) \exp(ik_z z - i\omega t) \tag{1}$$

Substituting Eq. (1) into the Maxwell's equations, we can write down the following equation

$$(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - \kappa_i^2) \overrightarrow{E}(x, y) = 0, \tag{2}$$

where

$$\kappa_0^2 = k_z^2 - \frac{\omega^2}{c^2} \tag{3a}$$

$$\kappa_i^2 = k_z^2 - \varepsilon_i(\omega) \frac{\omega^2}{c^2}, \quad (i = 1, 2)$$
(3b)

We will assume that the x- and y-component of the electric field E are independent of each other, i.e. $\overrightarrow{E}(x, y) = \overrightarrow{E}_x(x) \overrightarrow{E}_y(y)$, then Eq. (2) can be written as

$$\frac{1}{E_x(x)} \frac{d^2 E_x(x)}{dx^2} + \frac{1}{E_y(y)} \frac{d^2 E_y(y)}{dy^2} - \kappa_i^2 = 0$$
 (4)

and $E_x(x)$ and $E_y(y)$ are satisfied with the following equations, respectively

$$\frac{d^2 E_X(X)}{dX^2} = \alpha_i^2 E_X(X),\tag{4a}$$

and

$$\frac{d^2E_y(y)}{dy^2} = \beta_i^2 E_y(y),\tag{4b}$$

where

$$\alpha_i^2 + \beta_i^2 = \kappa_i^2 \ (i = 0, 1, 2)$$
 (5)

Extending the electromagnetic theory used by Mills and Maradudin [8] to the freestanding TMC quantum well wire system, the α - and β -components of the electric field E are expressed by

$$E_{\alpha} = E_{\alpha}(x) \exp(ik_{z}z - i\omega t) \quad (\alpha = x, z)$$
 (6)

and

$$E_{\beta} = E_{\beta}(y) \exp(ik_z z - i\omega t) \quad (b = y, z)$$
 (7)

where

$$E_{x}(x) = \begin{cases} A^{(0)} \exp(-\alpha_{0}x) & x > d_{2} \\ A^{(1)} \exp(\alpha_{2}x) + B^{(1)} \exp(-\alpha_{2}x) & d_{1} \le x \le d_{2} \\ A^{(2)} \exp(\alpha_{1}x) + B^{(2)} \exp(-\alpha_{1}x) & -d_{1} \le x \le d_{1} \\ A^{(3)} \exp(\alpha_{2}x) + B^{(3)} \exp(-\alpha_{2}x) & -d_{2} \le x \le -d_{1} \\ A^{(4)} \exp(\alpha_{0}x) & x < -d_{2} \end{cases}$$
(6a)

$$E_{z}(x) = \begin{cases} \frac{ik_{z}}{\alpha_{0}} A^{(0)} \exp(-\alpha_{0}x) & x > d_{2} \\ -\frac{ik_{z}}{\alpha_{2}} \left[A^{(1)} \exp(\alpha_{2}x) - B^{(1)} \exp(-\alpha_{2}x) \right] & d_{1} \le x \le d_{2} \\ -\frac{ik_{z}}{\alpha_{1}} \left[A^{(2)} \exp(\alpha_{1}x) - B^{(2)} \exp(-\alpha_{1}x) \right] & -d_{1} \le x \le d_{1} \\ -\frac{ik_{z}}{\alpha_{2}} \left[A^{(3)} \exp(\alpha_{2}x) - B^{(3)} \exp(-\alpha_{2}x) \right] & -d_{2} \le x \le -d_{1} \\ -\frac{ik_{z}}{\alpha_{0}} A^{(4)} \exp(\alpha_{0}x) & x < -d_{2} \end{cases}$$
(6b)

and

$$E_{y}(y) = \begin{cases} A^{(0)} \exp(-\beta_{0}y) & y > d_{2} \\ A^{(1)} \exp(\beta_{2}y) + B^{(1)} \exp(-\beta_{2}y) & d_{1} \le y \le d_{2} \\ A^{(2)} \exp(\beta_{1}y) + B^{(2)} \exp(-\beta_{1}y) & -d_{1} \le y \le d_{1} \\ A^{(3)} \exp(\beta_{2}y) + B^{(3)} \exp(-\beta_{2}y) & -d_{2} \le y \le -d_{1} \\ A^{(4)} \exp(\beta_{0}y) & y < -d_{2} \end{cases}$$
(7a)

$$E_{z}(y) = \begin{cases} \frac{ik_{z}}{\beta_{0}} A^{(0)} \exp(-\beta_{0}y) & y > d_{2} \\ -\frac{ik_{z}}{\alpha_{2}} \left[A^{(1)} \exp(\beta_{2}y) - B^{(1)} \exp(-\beta_{2}y) \right] & d_{1} \le y \le d_{2} \\ -\frac{ik_{z}}{\alpha_{1}} \left[A^{(2)} \exp(\beta_{1}y) - B^{(2)} \exp(-\beta_{1}y) \right] & -d_{1} \le y \le d_{1} \\ -\frac{ik_{z}}{\alpha_{2}} \left[A^{(3)} \exp(\beta_{2}y) - B^{(3)} \exp(-\beta_{2}y) \right] & -d_{2} \le y \le -d_{1} \\ -\frac{ik_{z}}{\alpha_{0}} A^{(4)} \exp(\beta_{0}y) & y < -d_{2} \end{cases}$$

$$(7b)$$

In Eqs. (6) and (7), $A^{(i)}$ (i=0,1,2,3,4) and $B^{(i)}$ (i=1,2,3) describe the amplitudes of the electric fields. $\alpha_i(\beta_i)$ (i=0,1,2) are the decay constants of the surface and interface waves in the vacuum, material "1" and material "2", respectively, and both are real and positive to keep the waves decaying as they depart from the surfaces and interfaces.

Combining the Maxwell's equations and boundary conditions of electromagnetic field, the implicit dispersion equation of the surface and interface phonon-polaritons in the freestanding QWW system can be obtained as

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