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ELECTRON RAMAN SCATTERING IN PYRAMIDAL QUANTUM DOTS

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ABSTRACT

The Raman scattering related with electrons in pyramidal quantum dots is theoretically investigated. The electron Raman differential cross section is calculated making use of analytically determined quantum states within the effective mass approximation. The features of the Raman differential cross section are discussed in terms of their dependence on the changes of the quantum dot geometry.

KEYWORDS: Quantum dots; Raman scattering; Pyramids; Conduction band; GaAs; Semiconductors.

DISPERSIÓN RAMAN DE ELECTRONES EN PUNTOS CUÁNTICOS PIRAMIDALES

RESUMEN

En este artículo se investiga teóricamente la dispersión Raman de electrones en puntos cuánticos piramidales. Se reporta la sección transversal diferencial Raman electrónica usando los estados cuánticos determinados analíticamente dentro de la aproximación de masa efectiva. Las características de la sección transversal diferencial Raman se discuten en términos de su dependencia de los cambios de la geometría de punto cuántico.

PALABRAS CLAVE: Puntos cuánticos, dispersión Raman, pirámides, banda de conducción, GaAs, semiconductores.

ESPALHAMENTO RAMAN DO ELÉTRONES EM PONTOS QUÂNTICOS PIRAMIDAIS

RESUMO

Este artigo busca pesquisar teoricamente o espalhamento Raman de elétrones em pontos quânticos piramidais. Reporta a seção transversal diferencial eletrônica de Raman usando estados quânticos determinados analiticamente dentro da aproximação de massa efetiva. As características da secção transversal diferencial de Raman são discutidos em termos de sua dependência das alterações da geometria do ponto quântico.

PALAVRAS-CHAVE: Pontos quânticos; Espalhamento Raman; Pirâmides; Banda de condução; GaAs; Semicondutores

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1. INTRODUCTION

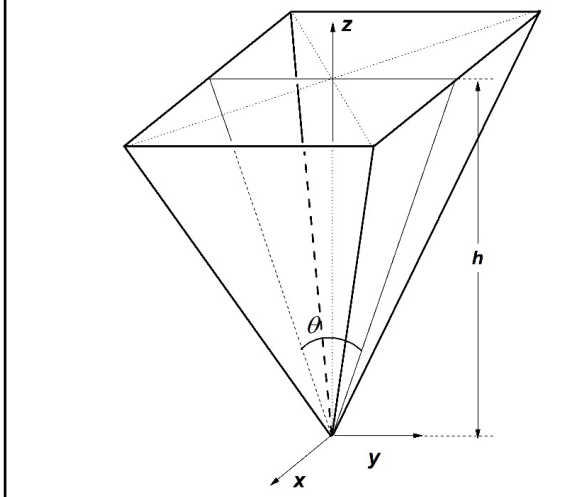
Semiconductor pyramidal quantum dots have been the object of study during much of the past two decades. These studies have demonstrated their potential for applications in the areas of optoelectronics and quantum information (see, for example, Pelucchi, *et al*. (2012) and references found there).

Over the years a larger number of theoretical and experimental articles on the electronic and optic properties of pyramidal quantum dots (QDs) have appeared in related literature Chaganti and Apalkov (2013). The calculation of the quantum states of load carriers in these types of systems has principally been occupied by the numeric solution to the differential equations in the approximation of mass effect, which has made research into different physical properties possible Park, Hong & Kim (2015). In the case of QDs there are reports of an analytic treatment of electronic states Lozovski & Piatnytsia (2011).

On the other hand, the study of the Raman scattering of electrons (in Spanish, *dispersión Raman de electrones* or DRE) in semiconductor heterostructures with low dimensionality dates back to the 1980s. In volume systems the treatment of the Raman scattering of electrons was first reported by Comas, Trallero-Giner & Pérez-Alvarez (1986). Soon after, the same phenomenon was reported as the case of quantum wells Riera, *et al*. (1988). Later, research rapidly expanded to other heterostructures like quantum threads and dots Betancourt-Riera, *et al* (2012). However, to the best of our knowledge, no research has been done on the characteristics of the Raman scattering of electrons in pyramidal quantum dots to date.

This article presents a study on the inelastic scattering of light, implying electronic transitions between different states in pyramidal QDs. The confined electronic states will be described through the analytical focus proposed by Lozovski & Piatnytsia (2011). In particular, the geometric influence of the pyramidal QDs on the Raman electron spectrum is studied. The article is organized in the following manner: Section 2 provides certain key elements of the theoretical model; Section 3 is devoted to presenting and discussing the results obtained; and Section 4 contains the conclusions.

Figure 1. Diagram of the pyramidal quantum dot analyzed in this study. The pyramid has a square base, a heigh (*h*), and an apical angle (θ). The potential for confinement is zero inside of the quantum dot and infinite in all other regions of the space



2. THEORETICAL FRAMEWORK

Figure 1 shows the pyramidal QD used within the analytic model to discover the electron states confined in the heterostructure. The system study focuses on an electron confined in a pyramidal region with a square base, a height (h), and an apical angle (θ). In the approximation of the effective mass the Schrödinger equation is given

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(\vec{r}) \right] \Psi(\vec{r}) = E\Psi(\vec{r}) \qquad (1)$$

where m^* is the effective mass of the electrons and $V(\vec{r})$ is the confinement potential defined as zero within the pyramidal QD and infinite in allother regions of the space. These $\Psi(\vec{r})$ are the eigenfunctions of the Hamiltonian with their corresponding eigenvalues E.

Following the work of Lozovski & Piatnytsia (2011) and considering the height of the pyramids as sufficiently large with respect to the side of the base (a situation one may arrive at with an apical angle of 60 degrees), the eigenfunctions for a confined electron in a pyramidal QD are given by

$$\Psi_{n,m,l}(\vec{r}) = N \frac{1}{\sqrt{z}} J_\theta(k_l z) [\sin(k_n/a) \cos(k_n x/z) + \cos(k_n/a) \sin(k_n x/z)] \times [\sin(k_m/a) \cos(k_m y/z) + \cos(k_m/a) \sin(k_m y/z)] \quad (2)$$

where $\theta = \sqrt{k_n^2 + k_m^2 + 1/4}$, $k_l h$ is the l-zero of the Bessel function, and N is a constant that guarantees normalization of the wave function. Additionally, $k_n = n\pi a / 2$ and $k_m = m\pi a / 2$ with $a = 1 / \tan(\theta / 2)$, and $n,m = 1,2,3,...$

The general expression for the differential cross section of the Raman scattering of electrons is given by Enderlein (1995)

$$\frac{d^2\sigma}{d\Omega\, dv_s} = \frac{V^2 v_s n(v_s)}{8\pi^3 c^4 n(v_L)} W(v_s, \hat{u}_s) \quad (3)$$

where c is the speed of light in a vacuum, $n(v)$ is the refractive index as a function of radiation frequency, $\hat{u}_s$ is the polarization vector of the secondary radiation frequently emitted, v_s, V is the pyramid volume, and v_L is the frequency of incident radiation whose polarization vector is $\hat{u}_L$. $W(v_s, \hat{u}_s)$ is the odds ratio for the transition, given by

$$W(v_s, \hat{u}_s) = \frac{2}{\hbar} \sum_{f=2}^{4} \left| \frac{\langle f | H_s | f+1 \rangle \langle f+1 | H_L | 1 \rangle}{E_s + E_f - E_{f+1} + i\Gamma_{f+1}} \right|^2 \frac{\Gamma_f}{(E_L - E_s + E_1 - E_f)^2 + \Gamma_f^2} \quad (4)$$

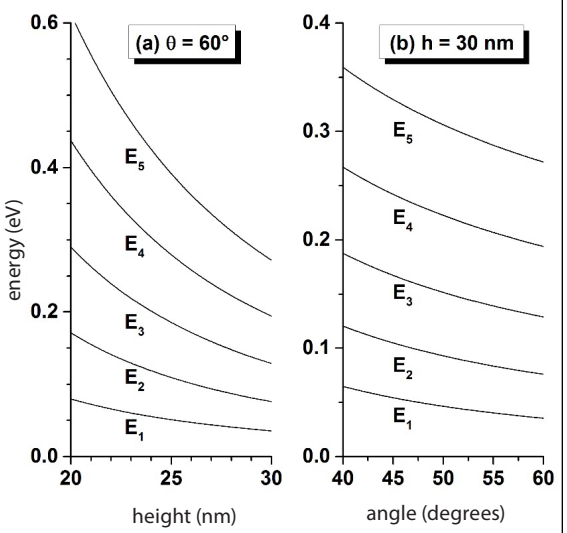
In this study only scatter processes involving contributions of transitions from the initial state $|1\rangle = \Psi_{1,1,1}(\vec{r})$ with energy $E_{1,1,1}$ to three final states $|l\rangle = \Psi_{1,1,l}(\vec{r})$ with energy $E_{1,1,,l}$ and $l = 2,3,4$ were considered. For interim states only the state $|l+1\rangle = \Psi_{1,1,l+1}(\vec{r})$ was included.In the case of line broadening for the interim and final states a fixed value of $\Gamma_{f+1} = \Gamma_f = 1.5 meV$ was chosen.

Given that the growth direction of the heterostructure is along the axis and the polarization of the incident and secondary radiation are also along the same axis, the electron-photon interaction operators that appear in the matrix elements of the transition odds ratio (H_k with $k = L,S$) are given by

$$H_k = \frac{i|e|}{m_0} \sqrt{\frac{2\pi\hbar^3}{V v_k}} \frac{\partial}{\partial z} \quad (5)$$

where m_0 is the free electron mass.

Figure 2. Variation of the energies $E_{1,1,l}$ with $l = 1,2,3,4,5$ 2(a) is based on the height of the pyramidal quantum dot for a fixed angle $\theta = 60°$, and 2(b) is based on the apical angle with a fixed height $h = 30\ nm$



3. RESULTS AND DISCUSSION

Figure 2a contains the energy variation $E_{1,1,,l}$ with $l = 1,2,3,4,5$ based on the height of the pyramidal QD, where $\theta = 60°$. Meanwhile **Figure 2b** shows the same five energies based on the apical angle where $h = 30\ nm$.

The decreasing behavior of the energies that appear in **Figure 2a** is a consequence of the progressive loss of the wave function localization due to the increase in size of the quantum dot. The same argument explains the variation in energy values shown in **Figure 2b**, although it is less pronounced given the conditions for the growth of $V(\vec{r})$ as it relates to the apical angle.

Figure 3. Variation of the product of the matrix elements for speed $T_{ijk} = \langle k|\partial/\partial z|j\rangle\langle j|\partial/\partial z|i\rangle$ for the states considered in Figure 2 based on the height of the pyramidal QD for a fixed angle $\theta = 60°$ (a) and on the apical angle with $h = 30\ nm$ (b).

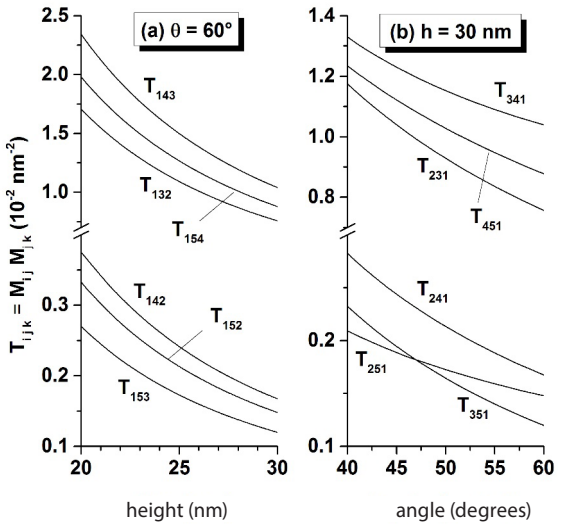


Figure 4. Variation of the differential cross section for the Raman scattering based on the secondary photon energy where $\theta = 60°$ with two values for the height of the pyramidal QD. The incident photon energy is fixed at 400 *meV*.

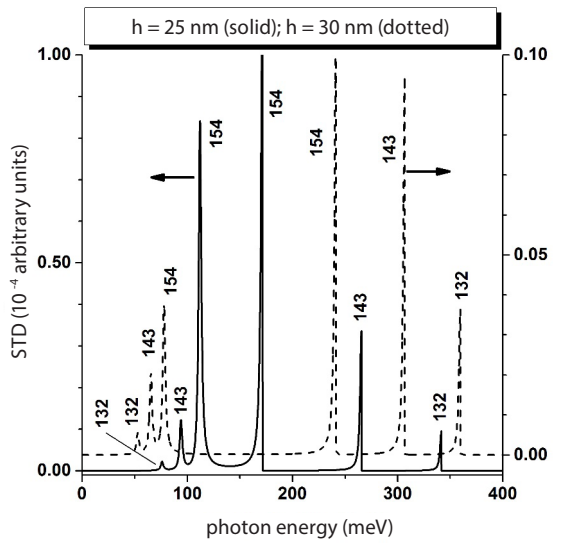


Figure 3 shows the product of the matrix elements for speed $T_{ijk} = \langle k|\partial/\partial z|j\rangle\langle j|\partial/\partial z|i\rangle$ for the states considered in **Figure 2**, based on the height of the pyramidal QD for a fixed angle $\theta = 60°$ 3(a) and on the apical angle with a fixed height $h = 30\ nm$ 3(b). Clearly the decreasing behavior of the aforementioned quantities has principally to do with the evolution of the spatial overlapping of the corresponding wave functions and their derivatives along the growth direction of the heterostructure.

With the information presented in **Figures 2** and **3** it is possible to evaluate the differential cross section of the Raman scattering related to the electrons that involve the five states mentioned in **Figure 2**. This amount appears in **Figure 4** for three configurations of initial-intermediate-final states chosen in particular, where $\theta = 60°$ and with two values for the height of the pyramidal QD. The differential cross section for the same processes are shown in **Figure 5**, having a fixed value of $h = 30\ nm$ and two different values for the apical angle. In both cases, the incidental photon energy is fixed at 400 *meV*.

The spectrums in both figures are the result of the sum of three processes where the same initial state is always utilized $|1\rangle$: $|1\rangle\rightarrow|3\rangle\rightarrow|2\rangle$ + $|1\rangle\rightarrow|4\rangle\rightarrow|3\rangle$ + $|1\rangle\rightarrow|5\rangle\rightarrow|4\rangle$. Note the appearance of resonance structures found at low energy with a symmetrical character, while those at high energy appear to have a step function structure with an asymmetrical character. The first resonance structures correspond to the condition $E_s = \hbar\omega_s = E_{f+1} - E_f$, while the step function structures correspond to the condition $E_s = \hbar\omega_s = \hbar\omega_L + E_1 - E_f$.

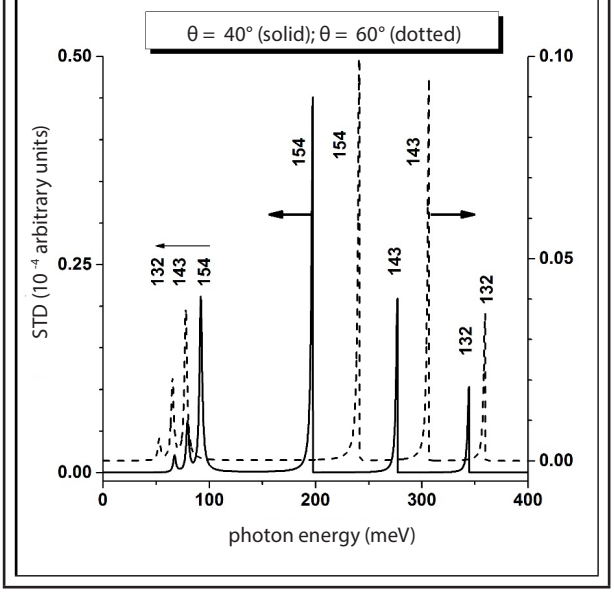


Figure 5. Variation of the differential cross section for Raman scattering in a scattered photon energy function where h = 30 *nm* with two different values for the apical angle. The incident photon energy is fixed at 400 *meV* .

It is possible to note that for the values greater than h, the step function structures scatter towards higher energies due to the decrease in values for the energy difference $E_f - E_1$, which is readily evident upon observing **Figure 2a**. The same thing happens when θ increases, although the blue current is less pronounced. In this case, the results represented in **Figure 2b** provide the explanation. The reason for the displacement into the red exhibited by the resonance structures is the same as previously mentioned. That is to say, the reduction in the energy difference $E_{f+1} - E_f$ as a consequence of the increase in the height of the quantum dot and of the apical angle. Furthermore, a reduction in the peak amplitude can be observed in both the function and resonance structures as a result of an increase in the values h and θ. To illustrate this situation, the dominant character can be attributed to the matrix elements for speed presented in **Figure 3**.

4. CONCLUSIONS

In this article the Raman scatter of electrons in pyramidal quantum dots with GaAs bases was researched. As determined by the use of an analytical approach, the electronic transitions exist between confined states. From among the states permitted one can choose a group with which to calculate the differential cross section for the Raman scatter, and further explore the effects had on it when changing the geometry by varying the height of the quantum dot and the size of the apical angle.

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