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First-order Raman scattering in cylindrical wurtzite nanowire

F. Lu, C.H. Liu *

College of Physics and Electronic Engineering, Guangzhou University, Guangzhou 510006, PR China

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ABSTRACT

We have presented a theoretical study on electron resonant Raman scattering (ERRS) process associated with the bulk longitudinal optical (LO), surface optical (SO) and quasi-confined (QC) phonon modes in a free-standing wurtzite nanowire (NW). We consider the Fröhlich electron–phonon interaction in the framework of the dielectric continuum model. Numerical calculations on the GaN material reveal that differential cross-section (DCS) is sensitive to the wire size. The bulk LO and high-frequency quasi-confined (QC_+) phonons make main contributions to the DCS and the impact of the SO phonon can be negligible in the ERRS process. Moreover, scattering intensity of the bulk LO phonon is strongly enhanced as the incident photon energy approaches the energy band-gap of the GaN.

1. Introduction

In the last decade, quasi-one-dimensional nanosemiconductors have attracted much attention for their significance in physics, and for their use as light emitters and detectors [1,2]. Known as an important III–V semiconductor, GaN nanowire (NW) is characterized by wurtzite structure and large-direct-band gap ($E_g = 3.4$ eV), which make the GaN NW a promising candidate for fabricating light-emitting diodes (LED) in the blue and green spectrum regions [3]. Besides those in optical devices, applications in high-power and high-frequency electronic devices have also attracted much attention since the GaN NW displays relatively high electron saturation velocity (2.5×10^2 cm/s) and high breakdown field (5×10^6 V/s), which is about three times larger than that of Si [4].

It is important to study such systems in order to determine their properties, and predict their behavior. Raman scattering measurement, being convenient and non-destructive, has been proven to be an ideal tool for studying various aspects of solids such as lattice and magnetic properties. In particular, the electronic structure can be studied through Raman scattering processes considering different polarizations of incident and emitted radiation [5,6]. Experimental researches on the Raman scattering in the GaN NW have been extensively reported [7–9]. Giehler et al. [7] analyzed the vibration properties of GaN by Raman spectroscopy, and demonstrated that the frequencies of two branches QC modes shift towards the corresponding A_1(LO) and E_1(LO) modes. Dhara et al. [10] discussed multiphonon Raman scattering in the GaN NW, and proved that the Fröhlich interaction gave rise to enhancement in the LO phonon modes. In order to explain the experimental results, many theoretical studies are focused on differential cross-section (DCS) for the Raman scattering process due to peak position and peak width of the Raman band can provide direct information concerning the electronic structure and phonon. Thus, the calculation of the DCS remains a fundamental work. Behr et al. [11] investigated the resonant Raman scattering in GaN/AlN single quantum well. The results show that the scattering intensity (SI) of the LO phonon is sorely enhanced as the incident photon energy approaches the energy band-gap of GaN. Considering built-in electric field effect, Lu et al. [12] studied the Raman scattering process without phonon in InGaN/GaN couple quantum wells. Liu et al. [13,14] calculated the first-order Raman scattering process in quantum discs and quantum wires. The Raman spectra they obtained give the direct information about the longitudinal optical (LO) and interface optical (IO) phonons respectively. However, the Raman spectra of the quasi-one dimensional GaN NW shows a new phonon mode, namely, quasi-confined phonon mode (QC) [15,16]. The QC phonon mode, a mixture of the LO and transverse (TO) modes, is separated from optical phonon modes in the cubic phase and uniquely related to the hexagonal phase. To the best of our knowledge, the electron–phonon interaction plays an important role in the scattering process because Raman scattering occurs essentially as a result of modulation of the electronic polarizability induced by various elementary excitations in solids such as phonon and plasmon [17,18]. Therefore, it is worthy of investigating the impact of the QC phonon on the DCS.

The organization of this paper is as follows. In Section 2, within the framework of the effective-mass approximation, the derivations

* Corresponding author. Tel.: +86 13342885677; fax: +86 20 39366871.
E-mail address: chliu64@yahoo.com.cn (C.H. Liu).

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of electronic eigenfunction and eigenvalue are presented. In Section 3, the analytical formula of the DCS is deduced under third-order perturbation approximation. In Section 4, the DCS as a function of radius is depicted and reasons are given in detail. Conclusions are presented in the last section.

2. Model and theory

The general 1D material system we consider are illustrated in Fig. 1. The z-direction is taken to be along the c-axis direction of the wurtzite crystal and the radial-(axial-) direction is denoted as t (z). The total Hamiltonian of the system can be written as follows:

$$\begin{aligned}\hat{H} &= \hat{H}_0 + \hat{H}_I \\ &= \hat{H}_e + \hat{H}_{ph} + \hat{H}_{e-ph}.\end{aligned} \tag{1}$$

$\hat{H}_e$ and $\hat{H}_{ph}$ denote the electron and phonon Hamiltonian, respectively. $\hat{H}_{e-ph}$, which describes the electron–phonon interaction, is considered as perturbation Hamiltonian H_I, while $\hat{H}_e+\hat{H}_{ph}$ is the unperturbation Hamiltonian H_0.

$$\hat{H}_e = \frac{\hbar^2}{2m^*}\nabla^2 + V(r), \tag{2}$$

with

$$V(r) = \begin{cases} 0 & r \le R, \\ \infty & r > R. \end{cases} \tag{3}$$

Within the framework of the dielectric continuum approximation the second and the third term in the right-hand side of Eq. (1) are

$$\hat{H}_{ph} = \hat{H}_{LO} + \hat{H}_{QC_\pm} + \hat{H}_{SO}, \tag{4}$$

$$\hat{H}_{e-ph} = \hat{H}_{e-LO} + \hat{H}_{e-SO} + \hat{H}_{e-QC_+} + \hat{H}_{e-QC_-}. \tag{5}$$

Here, the Fröhlich electron–phonon interaction can be written as [19]

$$\hat{H}_{e-QC_\pm,SO} = -e\sum_{m,k_z} \Gamma_{m,k_zR}^{QC_\pm,SO}(r)[b_m(k_z)e^{im\phi}e^{ik_zz} + h.c], \tag{6}$$

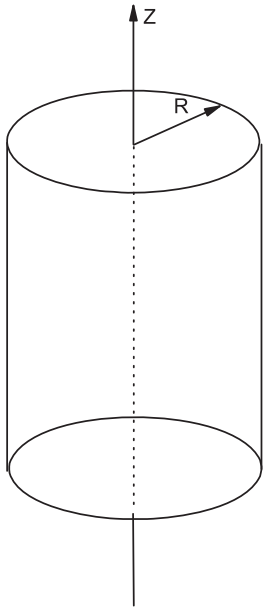

Fig. 1. A diagram of GaN quantum nanowire.

$$\hat{H}_{e-LO} = -e\sum_{m,k_z} \Gamma_m^{LO}(k_z)\left[a_m(k_z)J_m\left(\frac{\chi_{ml}}{R}r\right)e^{im\phi}e^{ik_zz} + h.c\right], \tag{7}$$

with

$$\Gamma_{m,k_zR}^{QC_\pm,SO}(r) = N_m(k_z)\begin{cases} K_m(k_zR)f_m(\gamma k_zr), & r \le R, \\ f_m(\gamma k_zR)K_m(k_zr), & r > R, \end{cases} \tag{8}$$

$$|\Gamma_m^{LO}(k_z)|^2 = \frac{4e^2\hbar\omega_{LO,t}}{L_zJ_{m+1}^2(\chi_{ml})\left[\chi_{ml}^2\left(\frac{1}{\varepsilon_{\infty,t}}-\frac{1}{\varepsilon_{0,t}}\right)^{-1} + R^2k_z^2\left(\frac{1}{\varepsilon_{\infty,z}}-\frac{1}{\varepsilon_{0,z}}\right)^{-1}\right]}, \tag{9}$$

$$\begin{aligned}|N_m(k_z)| = \sqrt{\frac{4\hbar\omega e^2}{k_z^2R^2L_z}}K_m^{-1}(k_zR)\{&\gamma^2\bar{\varepsilon}_t[f_{m+1}^2(\gamma k_zR) + f_{m-1}^2(\gamma k_zR) \\ &- f_m(\gamma k_zR)[f_{m+2}(\gamma k_zR) + f_{m-2}(\gamma k_zR)] + 2\bar{\varepsilon}_z[f_m^2(\gamma k_zR) \\ &- f_{m-1}(\gamma k_zR)f_{m+1}(\gamma k_zR)]]\}^{-1/2},\end{aligned} \tag{10}$$

and

$$f_m(\gamma k_zr) = \begin{cases} J_m(\gamma k_zr), & QC_\pm, \\ I_m(\gamma k_zr), & SO, \end{cases} \tag{11}$$

$$\gamma = \sqrt{\left|\frac{\varepsilon_z(\omega)}{\varepsilon_t(\omega)}\right|}. \tag{12}$$

k_z is the phonon wave number in the z direction. $J_m(x)$ is the Bessel function. $I_m(x)$ ($K_m(x)$) is the first- (second-) kind modified Bessel function. $\varepsilon_t(\omega)$ and $\varepsilon_z(\omega)$ are the dielectric functions in the directions along and perpendicular to the c-axis of the system. χ_{ml} is the lth zero root of the Bessel function $J_m(x)$. $\bar{\varepsilon}_\nu$ is the effective dielectric function given by

$$\bar{\varepsilon}_\nu = \left(\frac{1}{\varepsilon_\nu - \varepsilon_{\nu 0}} - \frac{1}{\varepsilon_\nu - \varepsilon_{\nu\infty}}\right), \quad \nu = t,z. \tag{13}$$

$\varepsilon_{\nu 0}$ and $\varepsilon_{\nu\infty}$ are, respectively, the static and high-frequency dielectric constants in the ν direction.

The solution of the Schrödinger equation is

$$\Psi_{ML}(r,\phi,z) = C_{ML}J_M\left(\frac{\chi_{ML}}{R}r\right)\exp(iM\phi)\exp(iK_zz). \tag{14}$$

C_{ML} is the normalized constant. χ_{ML} is the Lth zero root of the Bessel function $J_M(x)$. The corresponding eigenvalue is

$$\varepsilon_{ML}(K_z) = \frac{\hbar^2\chi_{ML}^2}{2m^*R^2} + \frac{\hbar^2K_z^2}{2m^*}. \tag{15}$$

The unperturbated wavefunction is

$$|M,L,K_z,n_{LO},n_{QC_\pm},n_{SO}\rangle = \Psi_{ML}(r,\phi,z)|n_{LO}\rangle|n_{QC}\rangle|n_{SO}\rangle. \tag{16}$$

n_{LO}, $n_{QC_\pm}$ and n_{SO} denote the LO, $QC_\pm$ and SO phonon numbers, respectively. Hence, the total energy of the electron–phonon system can be written as

$$E = \varepsilon_{ML}(K_z) + \sum_{n_{LO}}\hbar\omega_n(q_z)n_{LO} + \sum_{n_{QC_\pm}}\hbar\omega_n(q_z)n_{QC_\pm} + \sum_{n_{SO}}\hbar\omega_n(q_z)n_{SO}. \tag{17}$$

3. Differential cross-section

The general expression of the DCS is given by the third-order perturbation theory [20]

$$\frac{d^2\sigma}{d\omega_s d\Omega} = \frac{V^2\omega_s^2\eta(\omega_s)}{8\pi^3c^4\eta(\omega_l)}W(\omega_s,\vec{\mathbf{e}}_s). \tag{18}$$

c is the speed of light in free space. $\eta(\omega)$ is the refractive index as a function of the radiation frequency. $\vec{\mathbf{e}}_s$ is the polarization vector of the emitted secondary radiation field. Within the framework of the third-order perturbation theory, the transition matrix elements $W(\omega_s,\vec{\mathbf{e}}_s)$ from initial state $|i\rangle$ to final state $|f\rangle$ can