Confined-phonon effects in the band-gap renormalization of semiconductor quantum wires

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We calculate the band-gap renormalization in quasi-one-dimensional semiconductor quantum wires including carrier-carrier and carrier-phonon interactions. We use the quasistatic approximation to obtain the self-energies at the band edge that define the band-gap renormalization. The random-phase approximation at finite temperature is employed to describe the screening effects. We find that confined LO-phonon modes through their interaction with the electrons and holes modify the band gap significantly and produce a larger value than the static ϵ_0 approximation. [S0163-1829(98)01007-8]

I. INTRODUCTION

A dense electron-hole plasma being formed in a semiconductor under intense laser excitation comprises an interesting many-body system. Screening of the Coulomb interaction among the charge carriers renormalizes the single-particle properties. A notable phenomenon is the band-gap renormalization (BGR) as a function of the plasma density, which is important to determine the emission wavelength of coherent emitters as being used in semiconductors.[1] As a substantial amount of carrier population may be induced by optical excitation, the renormalized band gap can affect the excitation process in turn and lead to optical nonlinearities. In this paper we investigate the density dependence of the BGR in quasi-one-dimensional (Q1D) photoexcited semiconductors including the phonon effects. The band gap for 2D and bulk systems is found to decrease with increasing plasma density due to exchange-correlation effects. The observed band gaps are typically renormalized by ~ 20 meV within the range of plasma densities of interest, which arise chiefly from the conduction-band electrons and valence-band holes. In the Q1D structures based on the confinement of electrons and holes, the electron-hole plasma is quantized in two transverse directions, thus the charge carriers essentially move only in the longitudinal direction. Recent progress in fabrication techniques such as molecular-beam epitaxy (MBE) and lithographic deposition have made possible the realization of such quasi-one-dimensional systems.[2] Band-gap renormalization as well as various optical properties of the Q1D electron-hole systems have been studied[3–9] similar to the bulk (3D) and quantum-well (2D) semiconductors.[10–15] Some experimental results[9] indicate that the BGR in quantum wires is somewhat smaller than that predicted theoretically[4,5] and LO-phonon-carrier interaction effects to explain the discrepancy were suggested.[16] Polaronic corrections to the BGR were also investigated for quantum wells and quantum wires.[17]

One of our main motivations comes from the recent experiments[8] in which the carrier density dependence of a quasi-one-dimensional electron-hole plasma confined in GaAs quantum wires is investigated. Comparing the band-gap data with the available calculations, Cingolani *et al.*[8] pointed out the need for more realistic calculations. Density dependence of the BGR in Q1D systems was first considered by Benner and Haug[3] within the quasistatic approximation as previously employed for 2D and 3D systems.[10–13] Hu and Das Sarma[4] also calculated the BGR, neglecting the hole population and considering an electron plasma confined in the lowest conduction subband only. These results are in rather close agreement with the measurements,[8] although the analysis of experimental data was performed using a free-carrier model.

The aim of this paper is to study the carrier density dependence of the band-gap renormalization in quantum wires, when carrier-carrier and carrier-phonon interactions are included. We first show that for the quantum-wire model we use, the total band-gap renormalization is determined by the screened-exchange and Coulomb-hole contributions. We then demonstrate that within the quasistatic approximation to the self-energies, the explicit treatment of carrier-carrier and carrier-bulk phonon interactions does not reduce to the ϵ_0 approximation and gives a larger BGR. When the interaction of carriers with the confined phonon modes is considered, we obtain a similar magnitude for the BGR. We employ the dielectric continuum model[18] to describe the phonon confinement effects and incorporate the many-body renormalization effects due to electron-phonon interactions within our formalism. In low-dimensional semiconductor structures, phonon confinement is an essential part of the description of electron-phonon interactions. Since the early observation of confined phonons in GaAs/AlAs superlattices,[19] the phonon modes in microstructures have been attracting increasing attention.[20] Among the various macroscopic pictures, the dielectric continuum (DC) model[18,21] offers a simple framework to address the phonon confinement effects. The phonon modes in the DC model are (i) an infinite set of confined modes with vanishing electrostatic potentials at the interfaces which oscillate at the bulk LO-phonon frequency of GaAs, and (ii) a set of modes with electrostatic potentials attaining maxima at the interfaces. We include both the confined and interface phonon modes in our calculation, envisioning a thin wire of GaAs embedded in a barrier material of AlAs.

The rest of this paper is organized as follows. In the next section we give a brief outline of the static screening and quasistatic approximations. In Sec. III we present our results for the BGR in Q1D electron-hole plasmas interacting with LO phonons. Finally, we conclude with a brief summary of our main results.

II. MODEL AND THEORY

The quantum wire model we use is of cylindrical shape with radius R, and infinite potential barrier.[22] The quantum wire is made of material 1 (GaAs) and the surrounding material 2 (AlAs). Such a model leads to an analytic expression[22] $V(q)=(e^2/2\epsilon_0)F(q)$ for the Coulomb potential between the carriers within certain approximations. $F(q)$ is a form factor yielding $\sim\ln(qR)$ behavior in the long-wavelength limit, and ϵ_0 is the static dielectric constant (of material 1). The cylindrical wire model has the further advantage of treating the confined phonon modes in a simple way, as will be shown later. We assume that the linear plasma density N, is such that only the lowest subband is populated. This will hold[22] when the parameter $R_s=1/(2\pi NR)$, exceeds ~ 0.3. We assume that effective mass approximation holds and for GaAs take $m_e=0.067m$, and $m_h=0.5m$, where m is the bare electron mass. Due to the presence of an electron-hole plasma, assumed to be in equilibrium, the bare Coulomb interaction is screened. The equilibrium assumption is justified since the laser pulse durations are typically much longer than the relaxation times of the semiconductor structures under study. Defining the statically screened Coulomb interaction as $V_s(q)=V(q)/\varepsilon(q)$, we consider the dielectric function in the random-phase approximation (RPA)

$$\varepsilon(q)=1-2V(q)\sum_{i,k}\frac{f_i(k)-f_i(k+q)}{\epsilon_i(k)-\epsilon_i(k+q)+i\eta}, \qquad (1)$$

where the index $i=e,h$, and $\epsilon_i(k)=\hbar^2k^2/2m_i$ are the single-particle energies. Thus screening by both electrons and holes is accounted for within this approach. Assuming a homogeneously distributed electron-hole plasma in thermal equilibrium the electron and hole distribution functions are written as

$$f_i(k)=\frac{1}{e^{\beta[\epsilon_i(k)-\mu_i^0]}+1}, \qquad (2)$$

where $\beta=1/k_BT$ and μ_i^0 are the inverse carrier temperature and (unrenormalized) chemical potential of the different species, respectively. The plasma density N determines μ_i^0 through the normalization condition $N=2\Sigma_k f_i(k)$.

Adopting the quasistatic approximation,[10,11] which amounts to neglecting the recoil effects relative to the plasma frequency in the full frequency dependent expressions, we may decompose[10,11] the electron and hole self-energies into screened exchange (sx) and Coulomb hole (Ch) terms: $\Sigma_i(k)=\Sigma_i^{\mathrm{sx}}(k)+\Sigma_i^{\mathrm{Ch}}$, where

$$\Sigma_i^{\mathrm{sx}}(k)=-\sum_{k'}V_s(k-k')f_i(k'), \quad \text{and}$$

$$\Sigma_i^{\mathrm{Ch}}=\tfrac{1}{2}\sum_{k'}[V_s(k')-V(k')]. \qquad (3)$$

The above set of equations have been derived[10] from the dynamical self-energy expressions by neglecting all recoil energies with respect to the plasma frequency. As in the case of 2D and 3D calculations[10–14] we assume that the BGR results from rigid band shifts; i.e., the self-energies depend only weakly on wave vector k. The band-gap renormalization is then given by

$$\Delta E_g=E_g'-E_g=\Sigma_e(0)+\Sigma_h(0), \qquad (4)$$

namely, the electron and hole self-energies calculated at the respective band edges. Within the same spirit, we may calculate the renormalized total chemical potential of the electron-hole plasma using $\mu_T=\Sigma_i[\mu_i^0+\Sigma_i(k_F)]$, in which $k_F=\pi N/2$ is the Fermi wave vector. The self-energy part in the above expression is also called the exchange-correlation contribution μ_{xc} to the chemical potential.

In the case of the electron-phonon system, we take the bare Coulomb interaction to be $V(q)=(e^2/2\epsilon_{\infty 1})F(q)$ (note that the high-frequency dielectric constant of material 1, GaAs, is used) and include the phonon-mediated carrier-carrier interaction $V_{\mathrm{ph}}(q,\omega)=\Sigma_\lambda M_{q,\lambda}^2 D_\lambda(q,\omega)$ where the sum is over all the phonon modes present. Here M_q^2 is the effective 1D carrier-phonon matrix element, which depends on the type of phonon modes, and $D_\lambda(q,\omega)=2\omega_{\lambda,q}/(\omega^2-\omega_{\lambda,q}^2)$ is the phonon propagator, with phonon dispersion $\omega_{\lambda,q}$. The effective carrier-carrier interaction within the RPA is given by[23]

$$W(q,\omega)=\frac{V(q)+V_{\mathrm{ph}}(q,\omega)}{1-[V(q)+V_{\mathrm{ph}}(q,\omega)][\Pi_e(q,\omega)+\Pi_h(q,\omega)]}=\frac{V(q)}{\varepsilon_{\mathrm{TOT}}(q,\omega)}, \qquad (5)$$

where $\Pi_{e,h}(q,\omega)$ is the noninteracting density-density response function for electrons and holes [see also Eq. (1)]. The above equation defines the total dielectric function for the system in the presence of phonons, which can also be written as[23]

$$\varepsilon_{\mathrm{TOT}}(q,\omega)=\left[1+\frac{V_{\mathrm{ph}}(q,\omega)}{V(q)}\right]^{-1}-V(q)[\Pi_e(q,\omega)+\Pi_h(q,\omega)]. \qquad (6)$$

If the interaction of the charge carriers with the dispersionless bulk phonon modes in 1D is considered, with the matrix element $M_q^2=V(q)(1-\epsilon_\infty/\epsilon_0)\omega_{\mathrm{LO}}/2$, the static effective interaction $W(q,\omega=0)$ does not reduce to the ϵ_0-approximation result. This is when ϵ_∞ is replaced by ϵ_0 in the bare Coulomb interaction, and the carrier-phonon interactions are not included explicitly[24] ($V_{\mathrm{ph}}=0$). In our case the Coulomb-hole term contains the difference between the energy of the electron inside the plasma and in the semiconductor. Since we are in a quasistatic approximation the latter term contains ϵ_∞ not ϵ_0 as in the static ϵ_0 approximation.

Within the DC model, $V_{\rm ph}(q)$ is the sum of both the confined $V_{\rm ph}^{\rm conf}$ and all interface $V_{\rm ph}^{{\rm IF},n}$ mode potentials, which can interact in an electronic ground-state transition. The confined LO-phonon mode potentials in the wire are given by[21,25]

$$V_{\rm ph}^{\rm conf}(q,\omega)=\frac{e^2}{2\epsilon_{\infty 1}}\sum_n\left(1-\frac{\epsilon_{\infty 1}}{\epsilon_{01}}\right)\frac{\omega_{\rm LO1}[48J_3(x_{0n})/x_{0n}^3]^2}{J_1^2(x_{0n})(q^2R^2+x_{0n}^2)}\times\frac{2\omega_{\rm LO1}}{\omega^2-\omega_{\rm LO1}^2}. \quad (7)$$

In the above expression $J_n(x)$ is the Bessel function of order n, and x_{0n} is the nth root of $J_0(x)$. The interface phonon mode potential for mode n is[21,25]

$$V_{\rm ph}^{{\rm IF},n}(q,\omega)=\frac{e^2}{2\epsilon_{\infty 1}}\frac{\epsilon_{\infty 1}}{qRI_0(qR)I_1(qR)A(\omega_{qn})}\times\left[48\frac{I_3(qR)}{(qR)^3}\right]^2\frac{2\omega_{qn}}{\omega^2-\omega_{qn}^2}, \quad (8)$$

where

$$A(\omega)=\frac{\partial\epsilon_1(\omega)}{\partial\omega}-\frac{\epsilon_1(\omega)}{\epsilon_2(\omega)}\frac{\partial\epsilon_2(\omega)}{\partial\omega}, \quad (9)$$

and $\epsilon_{1,2}(\omega)$ are the GaAs (1) and AlAs (2) phonon dielectric functions, given by $\epsilon_i(\omega)=\epsilon_{\infty i}(\omega^2-\omega_{\rm LOi}^2/\omega^2-\omega_{\rm TOi}^2)$, ω_{qn} are the interface mode frequencies,[18] and $I_n(x)$ is the nth order modified Bessel function of the first kind. The confined phonons have the GaAs zone center frequency whereas the interface modes have dispersive frequencies which lie in the *reststrahl* band of the wire and barrier materials.[18] These are labeled as GaAs interface and AlAs interface modes depending on their frequency. Only the lowest-order confined and interface modes interact in a one-subband approximation. A more detailed description of DC phonon modes interacting with Q1D electrons is given by Bennett *et al.*[21] and Wang and Lei.[25]

Finally, in the case of the electron-phonon system, we should subtract the polaronic renormalization (of the band edges) Δ_p from the band-gap renormalization ΔE_g, as was done for 2D systems,[24] since this is already included but cannot be measured by experiment. Δ_p is obtained from perturbation theory in the one carrier limit at zero temperature as

$$\Delta_B=-\frac{2}{\pi}\left(1-\frac{\epsilon_\infty}{\epsilon_0}\right)\omega_{\rm LO}\sum_{i=e,h}\int dq\frac{V(q)}{q^2/2m_i+\omega_{\rm LO}} \quad (10)$$

for bulk phonons and

$$\Delta_{\rm DC}=\frac{4}{\pi}\sum_{i=e,h}\left[\int dq\frac{V_{\rm ph}^{\rm conf}(q,0)}{q^2/2m_i+\omega_{\rm LO1}}+\sum_n\int dq\frac{V_{\rm ph}^{{\rm IF},n}(q,0)}{q^2/2m_i+\omega_{qn}}\right] \quad (11)$$

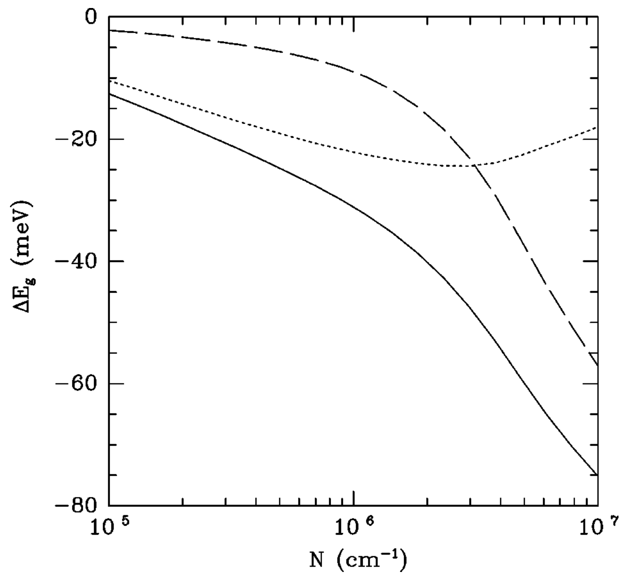

FIG. 1. The band-gap renormalization in the ϵ_0 approximation as a function of plasma density N, for a quantum wire of $R=50$ Å, and at $T=100$ K. The dashed and dotted lines indicate the screened-exchange and Coulomb-hole contributions, respectively, whereas the solid line stands for the total ΔE_g.

for DC phonons. Unlike in 3D and 2D systems, in 1D a closed form expression for Δ_p is not possible[17] because of the nature of the form factors contained in $V(q)$ and $V_{\rm ph}(q)$.

III. RESULTS AND DISCUSSION

We now present our results on the band-gap renormalization in Q1D quantum wires, concentrating on the density range of $N=10^5-10^7$ cm^{-1}. We first discuss the screened-exchange and Coulomb-hole contributions to the BGR without subtracting the polaronic renormalization. Figure 1 shows ΔE_g as a function of N for a quantum wire of $R=50$ Å, at $T=0$. We do not include the phonon effects explicitly, but use the ϵ_0 approximation for material 1 for the time being. The rationale for this approximation, as argued by Das Sarma, Jalabert, and Yang,[24] is that the effect of high-frequency phonons is to screen the Coulomb interaction, which is accounted for by the replacement of ϵ_∞ by ϵ_0. The dashed and dotted lines denote the screened-exchange and Coulomb-hole contributions, respectively, whereas the solid line is the total BGR. There are several noteworthy features. For the cylindrical quantum-wire model we use, the Coulomb-hole contribution is important in determining the total ΔE_g. In a different wire model, Benner and Haug[3] found the density dependence of ΔE_g is not as strong as ours, and it is mainly determined by the screened-exchange contribution. Our finding here is also in contrast with the situation in 2D and 3D systems, where the BGR is to a large extent determined by the Coulomb-hole contribution.[26] The slight upturn in the Coulomb-hole contribution at high densities is a peculiar effect, perhaps related to the 1D character of the system. Similar behavior was also found in a different quantum-wire model.[27] Since the analysis of the photoluminescence measurements depends on the theoretical model used to extract the observed BGR, a direct comparison with experimental data is difficult. However, it is conceivable to

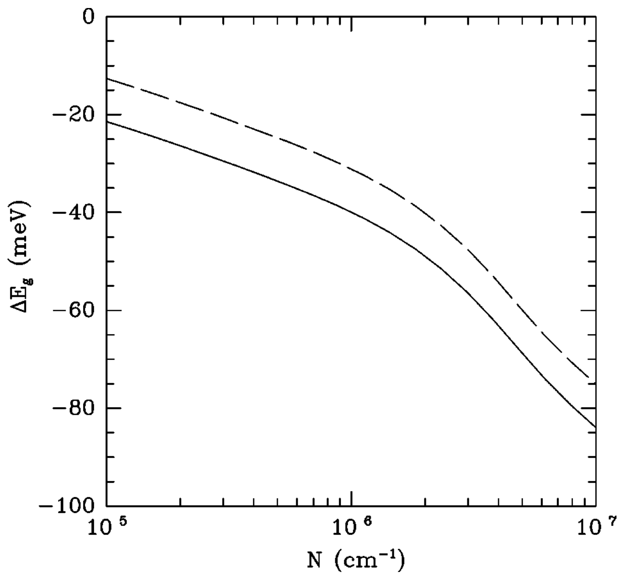

FIG. 2. The band-gap renormalization for a $R=50$ Å wire at $T=100$ K using the quasistatic approach with bulk GaAs phonons (solid) and the ϵ_0 approximation for material 1 (dashed).

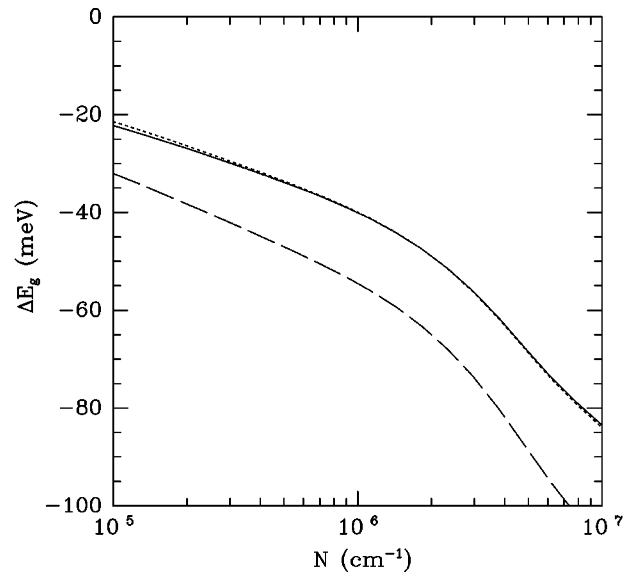

FIG. 3. The band-gap renormalization within the quasistatic approach including DC phonons (solid line), bulk GaAs phonons (dotted line), or bulk AlAs phonons (dashed line) with $R=50$ Å and $T=100$ K.

have drastically different N dependence for the BGR, depending on the degree of confinement as described by various models.

We next investigate the effects of carrier-phonon interaction on the BGR. For this purpose, the bare carrier-carrier- and carrier-phonon-mediated interactions should be treated on an equal footing. If one were to use the dynamically screened effective interaction within the RPA, the phonon effects would be discerned. In quantum-well systems, taking also the finite-width effects into account, Das Sarma, Jalabert, and Yang[24] have found that ϵ_0 approximation is sufficient to describe the phonon interaction effects for weakly coupled polar materials. However, the calculations of Das Sarma, Jalabert, and Yang[24] show that the phonon effects tend to increase the magnitude of BGR. Dan and Bechstedt[16] calculated the LO-phonon effects in Q1D systems, within the quasistatic approximation. They found that phonon effects reduce the magnitude of ΔE_g. We believe that this discrepancy partly stems from the fact that the static dielectric constant ϵ_0 appears in the Coulomb interaction, even though they treat the carrier-carrier and carrier-phonon interactions on an equal footing.

We compare the result of the ϵ_0 approximation and the result using the phonon potentials for bulk GaAs phonons in Fig. 2. Both results have the same form but using the quasistatic approximation gives a larger BGR because we have, at least in part, included some effect of a finite frequency. As discussed in the previous section, the self-energy in the semiconductor, which appears in the Coulomb hole term, still contains $\epsilon_{\infty 1}$. Our results indicate an increase in the magnitude of BGR upon the inclusion of explicit phonon effects similar to the situation[24] in 2D. Since our approach is not fully dynamical but quasistatic the effect may have been slightly overestimated and the true BGR lies between the two extreme results.

Using the phonon potentials for confined LO-phonon modes and interface phonon modes, we next calculate the BGR within the quasistatic approximation. Our results for a quantum wire of radius $R=50$ Å are shown in Fig. 3. The solid, dotted, and dashed lines represent ΔE_g calculated using carrier-DC phonon, carrier-bulk GaAs phonon, and carrier-bulk AlAs phonon interactions, respectively. Figure 4 shows the same curves against R with $N=10^6$ cm^{-1}. We assume confined LO phonons to be dispersionless, but use the dispersion relations for interface phonon modes derived within the DC model.[21,25] Also, we have not deducted the polaronic renormalization. The DC phonon result appears to lie very close to the bulk GaAs phonon result. This is in contrast to earlier works[28] and to the approximate sum rule,[29] which is known to hold for the DC model, namely, for small R the DC result should give the bulk AlAs phonon result and

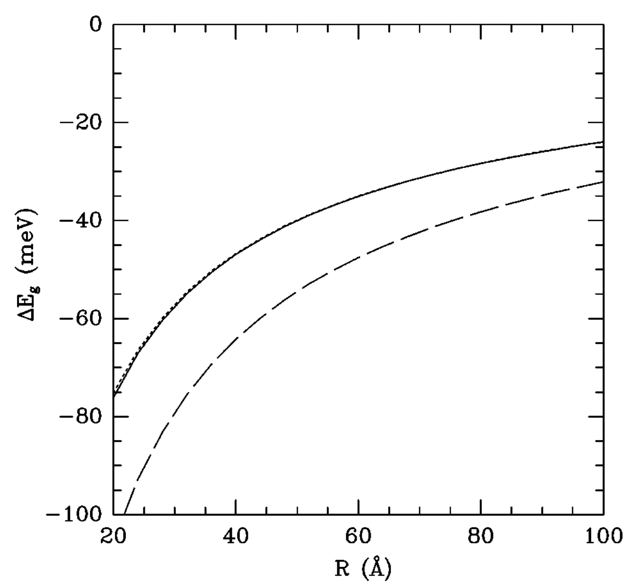

FIG. 4. The band-gap renormalization as a function of quantum wire radius within the quasistatic approach including DC phonons (solid line), bulk GaAs phonons (dotted line), or bulk AlAs phonons (dashed line) with $N=10^6$ cm^{-1} and $T=100$ K.

for large R the bulk GaAs phonon result. The phonon potentials *do* reduce to the bulk phonon results at the appropriate limits, however, the AlAs bulk limit is not reached because the dependence is on qR and the integration over q is infinite. This implies that in the quasistatic case the BGR is controlled by shorter wavelength modes than is usually the case. Thus, the result using DC phonons only reduces to the result with AlAs bulk phonons for very small radii.

Subtracting the polaronic effects leads to another interesting result. The polaron shift (Δ_{DC}) tends towards the small radius limit of the sum rule for the DC model for larger values of R than the quasistatic approximation. Thus, subtracting polaronic effects produces a result where the BGR including DC phonons is smaller than both of the bulk phonon cases. This does not contradict the approximate sum rule, since the result is the difference between the quasistatic approximation and polaronic shifts that independently satisfy the sum rule. Our results with polaronic shifts subtracted are illustrated in Fig. 5. The decrease in magnitude for all the cases is similar to that obtained by Das Sarma, Jalabert, and Yang[24] for 2D systems.

The main shortcoming of the present calculation is the quasistatic approximation employed to obtain the self-energies. However, the confined and interface phonon contributions to the BGR can be estimated. A more complete theory should take the full frequency dependence of the various phonon potentials which appear in the total dielectric function $\varepsilon(q,\omega)$, and perform an internal frequency integral, similar to the case in 2D systems.[14,24]

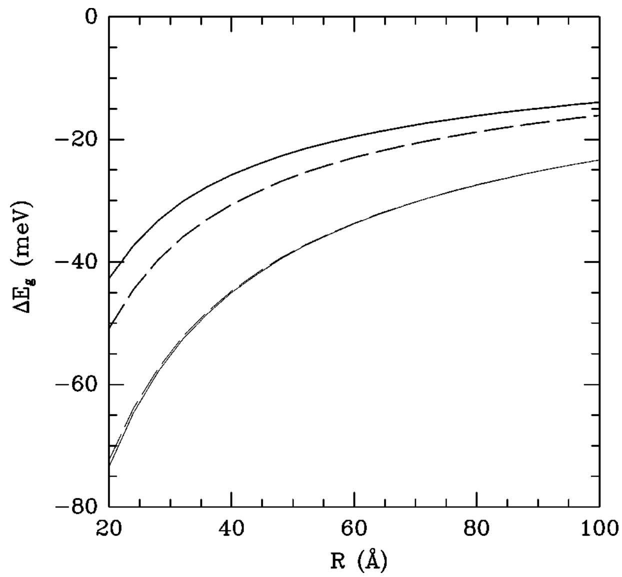

FIG. 5. The band-gap renormalization as a function of quantum wire radius within the quasistatic approach including DC phonons (solid line), bulk GaAs phonons (dashed line) with $N=10^6$ cm^{-1} and $T=0$ K. The thin curves are just the quasistatic result while the thick curves do not include the polaronic energy shift.

IV. SUMMARY

In this paper, we have examined the effects of carrier-phonon interactions on the band-gap renormalization in photoexcited Q1D semiconductor structures. Within the quasistatic approximation and the RPA, the carrier-bulk LO-phonon interactions are different from the ϵ_0 approximation and produce a larger BGR. The full dynamic result should lie between these two results. When we consider the confined LO-phonon modes and interface phonon modes, described within the dielectric continuum model, we find that the carrier-phonon interaction effects do not increase significantly the magnitude of the band-gap renormalization when compared to band-gap renormalization including bulk GaAs phonons. However, excluding the polaronic effects, which cannot be measured experimentally, a smaller BGR is obtained for the DC phonon modes than for the bulk phonons. Extension of our calculations to multisubband cases would be interesting.

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