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The polaron effects and temperature dependence of the strong-coupling exciton in slab of polar crystals

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Abstract. The system, in which the excitons interact with both the weak-coupling bulk longitudinal-optical (LO) phonons and strong-coupling surface-optical (SO) phonons in a slab of polar crystal, is studied by using a linear combination operator and the Lee-Low-Pines variational method. The expression of the induced potential of the exciton is derived, and the numerical calculations for the AgBr crystal as an example are made. The results show that the induced potential of the exciton relates not only to the distance between electron and hole, but also to the thickness of slab and temperature.

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Key words: exciton, strong-coupling, induced potential

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1 Introduction

The properties of the polar crystal slab, quantum well and superlattice and other low dimensional materials have aroused great interest [1-5] as the research object to the development of smaller size and dimension, and the materials to the multilayer film structure trend. In recent decades, many domestic and foreign researches on the low dimensional materials element excitation were carried out by many studies [6-12], especially the problems of exciton in a slab. In their study of the exciton in a slab, when the interaction of the exciton both with the surface-optical (SO) phonons and bulk longitudinal-optical (LO) phonons were considered, they mainly concentrated their attention on the weak and intermediate coupling case [13]. In fact, in some polar crystal, the coupling of the electrified particle with the surface or the interface optical phonons is strong, but weak with LO phonons [14]. Therefore, the research on the exciton system, in which the excitons interact with both the weak-coupling bulk LO-phonons and strong-coupling SO-phonons at finite temperature in a polar crystal slab, is more important.

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2 Theoretical method

Consider a slab of polar crystal with thickness $2d$. In the effective-mass approximation, the Hamiltonian of the exciton-phonon system in the polar slab can be written as [15]

$$H = H_{ex} + H_{ph} + H_{e-LO} + H_{e-SO} + H_{h-LO} + H_{h-SO} \tag{1}$$

$$H_{ex} = H_e + H_h + H_{e-h} \tag{2}$$

$$H_e = \begin{cases} \frac{p_{ez}^2}{2m_e} + \frac{p_e^2}{2m_e}, & |z_e| \le d \\ \frac{p_{ez}^2}{2m_0} + \frac{p_e^2}{2m_0} + V_0, & |z_e| > d \end{cases} \tag{2a}$$

$$H_h = \begin{cases} \frac{p_{hz}^2}{2m_h} + \frac{p_h^2}{2m_h}, & |z_h| \le d \\ \frac{p_{hz}^2}{2m_0} + \frac{p_h^2}{2m_0} + V_0', & |z_h| > d \end{cases} \tag{2b}$$

$$H_{e-h} = -\frac{e^2}{\varepsilon_\infty |r_e - r_h|} \tag{2c}$$

$$H_{ph} = H_{LO} + H_{SO} \tag{3}$$

$$H_{LO} = \sum_{k,m,p} a_{k,m,p}^{+} a_{k,m,p} \hbar\omega_{LO} \tag{3a}$$

$$H_{SO} = \sum_{q,p} b_{q,p}^{+} b_{q,p} \hbar\omega_{SO} \tag{3b}$$

$$H_{e-SO} = \sum_q \left(\frac{\sin(2qd)}{q}\right)^{\frac{1}{2}} e^{-qd} \left[C^* e^{-iq\cdot p_e} [G_+(q,z_e) b_{q,+}^{+} + G_-(q,z_e) b_{q,-}^{+}] + H.c.\right] \tag{4}$$

$$H_{h-SO} = -\sum_q \left(\frac{\sin(2qd)}{q}\right)^{\frac{1}{2}} e^{-qd} \left[C^* e^{-iq\cdot p_h} [G_+(q,z_h) b_{q,+}^{+} + G_-(q,z_h) b_{q,-}^{+}] + H.c.\right] \tag{5}$$

$$H_{e-LO} = \sum_k \left[B^* e^{-ik\cdot p_e} \left[\sum_{m=1,3,5\ldots} \frac{\cos(\frac{m\pi z_e}{2d})}{[k^2 + (\frac{m\pi}{2d})^2]^{\frac{1}{2}}} a_{k,m,p}^{+} + \sum_{m=2,4,6\ldots} \frac{\sin(\frac{m\pi z_e}{2d})}{[k^2 + (\frac{m\pi}{2d})^2]^{\frac{1}{2}}} a_{k,m,p}^{+} \right] + H.c. \right] \tag{6}$$

$$H_{h-LO} = -\sum_k \left[B^* e^{-ik\cdot p_h} \left[\sum_{m=1,3,5\ldots} \frac{\cos(\frac{m\pi z_h}{2d})}{[k^2 + (\frac{m\pi}{2d})^2]^{\frac{1}{2}}} a_{k,m,p}^{+} + \sum_{m=2,4,6\ldots} \frac{\sin(\frac{m\pi z_h}{2d})}{[k^2 + (\frac{m\pi}{2d})^2]^{\frac{1}{2}}} a_{k,m,p}^{+} \right] + H.c. \right] \tag{7}$$

In calculation, we introduce the mass centre coordinate and relative coordinate of exciton, then we also introduce the Huybrechts linear combination operator for the mass center momentum and mass center coordinate. In order to simplify the calculation, we apply two unitary transformations to the Hamiltonian, finally we discuss the extremum of the average value $\bar{H}$. The effective Hamiltonian for the exciton-phonon system is defined as the variation of $\bar{H}$ with respect to $f_{k,m,p}(f_{k,m,p})$, $g_{q,p}(g_{q,p})$, and λ, then it can be obtained as

$$H_{eff}=\frac{\pi^2\hbar^2 l_1^2}{8m_e d^2}+\frac{\pi^2\hbar^2 l_1^2}{8m_h d^2}+\frac{p^2}{2\mu}-\frac{\lambda_{\min}e^2}{\varepsilon_\infty \rho}+(n+\frac{1}{2})\hbar\lambda_0+\sum_{k,m,p}\hbar\omega_{LO}n_q+\sum_{k,m,p}\hbar\omega_{SO}n_q$$
$$+V_{IB}^{l_1 l_2}(\rho)+V_{IS}^{l_1 l_2}(\rho)+V_1^0(z_e)+V_1^0(z_h) \tag{8}$$

where $V_{IB}^{l_1,l_2}(\rho)$ and $V_{IS}^{l_1,l_2}(\rho)$ are the induced potential of exciton which is produced by the interaction between exciton and LO-phonons and SO-phonons respectively.

3 Numerical analysis and discussion

The calculations are described as follows. Fig. 1 shows the variation of the induced potential $V_{e,h-LO}$, produced by the interaction of the exciton and LO-phonon, with under conditions of different temperature and a certain thickness of the slab in AgBr polar crystal slab. From the figure, we can see that induced potential $V_{e,h-LO}$ will increase with decreasing ρ and decrease with increasing T. This is because with increasing the temperature, the lattice irregular motion enhancement, the weaker the interaction between electron (hole) and phonon.

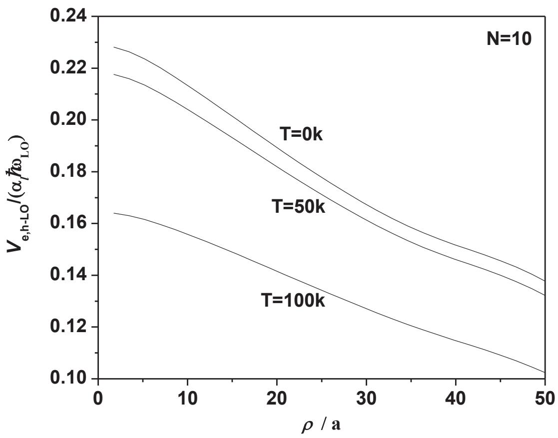

Figure 1: The relationship of the exciton induced potential $V_{e,h-LO}$, which is induced by the interaction between the exciton and LO-phonon, with the coordinate ρ and temperature T at $N=10$.

Fig. 2 describes the variation of the induced potential $V_{e,h-LO}$, which is produced by the interaction between the exciton and LO-phonon, with the distance ρ between the electron and hole at different thickness of the slab N and a certain temperature T in AgBr polar crystal slab. From the figure, we can see that the induced potential $V_{e,h-LO}$ will decrease with increasing ρ and increase with increasing N. It is indicated that the thicker the

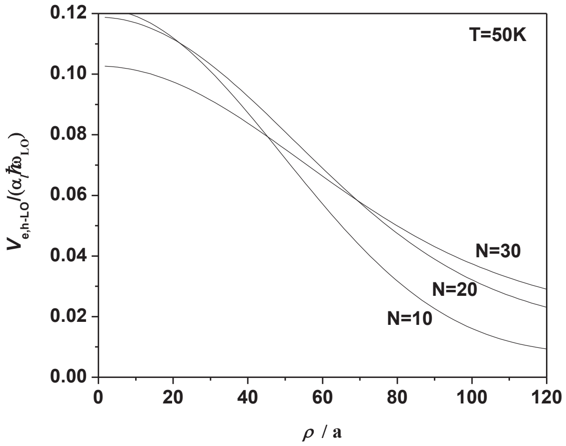

Figure 2: The relationship of the exciton induced potential $V_{e,h-LO}$, which is induced by the interaction between the exciton and LO-phonon, with the coordinate ρ and N at $T = 50$K.

slab, the stronger the interaction between the exciton and LO-phonons, the contribution of the exciton-LO phonon interaction to the induced potential is dominant.

Fig. 3 shows the relationship between the exciton induced potential $V_{e,h-SO}$, which is induced by the interaction between the exciton and SO-phonon, with the coordinate ρ and N at a certain temperature T in AgBr polar crystal slab. It can be seen from the figure that the induced potential $V_{e,h-SO}$ will decrease with increasing ρ and increase with decreasing N.

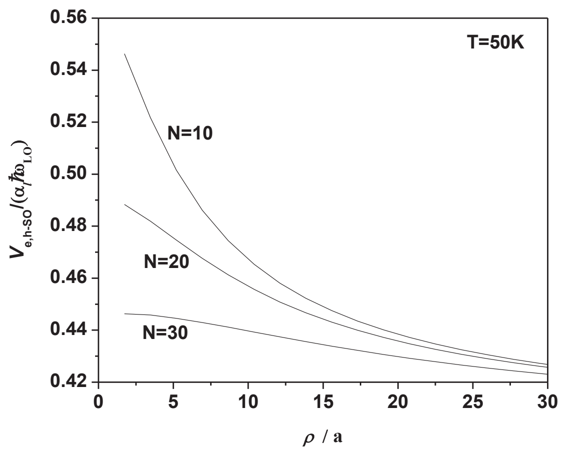

Figure 3: The relationship of the exciton induced potential $V_{e,h-SO}$, which is induced by the interaction between the exciton and SO-phonon, with the coordinate ρ and N at $T = 50$K.

4 Conclusions

In conclusion, we have investigated the system, in which the excitons interact with both the weak-coupling bulk LO phonons and the strong-coupling SO phonons in a slab of polar crystal, by using a linear combination operator and the Lee-Low-Pines variational method. Numerical calculations for the AgBr polar crystal slab show that the coupling intensity between exciton with different phonon in a polar crystal slab is different. At the same time, the influence of the temperature and the surface phonon on the induced potential can not be neglected.

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