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Size-Quantum Effect of the Energy of a Charge Carrier in a Semiconductor Crystallite

By

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The size-quantum effect of the energy of a charged carrier in a spherical semiconductor crystallite embedded in another spherical dielectric layer is discussed and the interaction of the charged carrier with surface optical (SO) and longitudinal optical (LO) vibrations is taken into account. In the first-order approximation of the energy the charged carrier does not interact with SO vibrations, and it interacts only with LO vibration of the dielectric in which the charged carrier is located. The interaction energy between the charged carrier and LO vibrations will increase with decreasing the size of crystallite.

Обсудили размерно-квантованное эффект энегрии зараженных частиц в сферических полупроводниковых микро-кристаллитах, находящиеся в другом сферическом диэлектрическом слое. В обсуждении также рассмотрили взаимодействие между заряженной частицей и SO и LO колебанями. В первой приближении энергии, заряженная частица не взаймодействует с SO колебанями, но только взаймодействует с теми LO колеьанями в диэлектрике, где она была. Взаймодействие энергии между заряженными частицами и LO колебанями возрастает с уменьщением размера кристаллитов.

1. Introduction

Recently, the size-quantum effect has been observed in commercial optical glass filters and other microcrystallites [1 to 3]. It was also reported that small CdS, ZnO, and other crystallites are synthesized via colloidal chemical techniques, and when the diameter of crystallite is lower than 5×10^{-9} m, the absorption edge is shifted to higher energy (blue shift) [4, 5]. At the same time, some theoretical works were presented in which the charge carrier in the crystallite is assumed to move in a spherical potential well, and the effective mass approximation is used [6, 7]. However, the considerations of different authors on the influence of the dielectric polarization are different. Thus, this problem is worth to be taken into consideration further.

In this paper, we will extend the theory of the electron–phonon interaction in dielectric bilayers [8] to a spherical crystallite embedded in another dielectric, and find out the interaction energy of the charge carrier with SO and LO vibrations. In calculating the energy of the charge carrier in the crystallite, the method developed by Pekar [9] for discussing the behaviour of a charged particle in alkaline halides is used. It is found that 1. the energy of the charge carrier in a crystallite rapidly increases with the decrease of the size of the crystallite, 2. in the first-order approximation of the energy the charge carrier in the crystallite does not interact with SO vibrations, 3. the inter-

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action energy of the charge carrier with LO vibrations is inversely proportional to the radius of the crystallite, R. It can be expected from this that the ionization and affinity potentials of the charged particle in the colloidal crystallite should show a size quantum effect, too. This property is important for the surface chemical and catalytic reactions.

2. Elementary Model and Theory

If spherical or other-shaped microcrystallites are randomly distributed in another medium, and their concentration is very low, such a system can be regarded as a single crystallite embedded in a large piece of a medium. For example, the optical glass containing Cd(S, Se) crystallites and the colloidal crystallites in liquid solution can be regarded as such a system. For simplifying the theoretical treatments, a spherical crystallite and only one mobile charge carrier (electron or hole) in it are assumed. In what follows we shall use the subscript $n = 1$ for the spherical crystallite, $n = 2$ for medium surrounding it. For a spherical crystallite with radius R embedded in another medium, the polarization strengths associated with SO and LO vibrations are [8], respectively,

$$\boldsymbol{p}_1^{\mathrm{so}}(\boldsymbol{r}) = \sum_{lm} C_{lm,1}^{\mathrm{so}} \boldsymbol{p}_{lm}^{\mathrm{so}}(\boldsymbol{r}) = \nabla_{\boldsymbol{r}} \sum_{lm} C_{lm,1}^{\mathrm{so}} \left(\frac{r^l}{R^{l+1}}\right) Y_l^m(\hat{r}) ; \qquad r < R , \tag{2.1a}$$

$$\boldsymbol{p}_2^{\mathrm{so}}(\boldsymbol{r}) = \sum_{lm} C_{lm,2}^{\mathrm{so}} \boldsymbol{p}_{lm,2}^{\mathrm{so}}(\boldsymbol{r}) = \nabla_{\boldsymbol{r}} \sum_{lm} C_{lm,2}^{\mathrm{so}} \left(\frac{R^l}{r^{l+1}}\right) Y_l^m(\hat{r}) ; \qquad r > R \tag{2.1b}$$

and

$$\boldsymbol{p}_1^{\mathrm{lo}}(\boldsymbol{r}) = \sum_{lm} C_{lm,1}^{\mathrm{lo}} \boldsymbol{p}_{lm,1}^{\mathrm{lo}}(\boldsymbol{r}) = \nabla_{\boldsymbol{r}} \sum_{lm} C_{lm,1}^{\mathrm{lo}} j_l(k_{ls} r)\, Y_l^m(\hat{r}) ; \qquad r < R , \tag{2.1c}$$

$$\boldsymbol{p}_2^{\mathrm{lo}}(\boldsymbol{r}) = \sum_{lm} C_{lm,2}^{\mathrm{lo}} \boldsymbol{p}_{lm,2}^{\mathrm{lo}}(\boldsymbol{r}) = \nabla_{\boldsymbol{r}} \sum_{lm} C_{lm,2}^{\mathrm{lo}} f_l(k_{ls} r)\, Y_l^m(\hat{r}) ; \qquad r > R , \tag{2.1d}$$

where $j_l(k_l r)$ is the spherical Bessel function, $f_l(k_l r)$ a linear combination of spherical Bessel and Neumann functions,

$$f_l(k_l r) = A j_l(k_l r) + B n_l(k_l r) . \tag{2.2}$$

For the SO vibration, the dispersion relation and the connection between $C_{lm,1}^{\mathrm{so}}$ and $C_{lm,2}^{\mathrm{so}}$ are obtained from the boundary conditions to be

$$\varepsilon_1(\omega^{\mathrm{so}}) = -(l+1)\, \varepsilon_2(\omega^{\mathrm{so}}) ; \qquad l = 1, 2, \ldots , \tag{2.3a}$$

$$C_{lm,1}^{\mathrm{so}} = -\left(\frac{x_1}{x_2}\right) C_{lm,2}^{\mathrm{so}} ; \qquad l = 1, 2, \ldots , \tag{2.3b}$$

where ε_n and x_n are the dielectric function and the susceptibility of the dielectric layer n, respectively.

For the LO vibration, we have from the boundary conditions

$$j_l(k_{ls} R) = 0 ; \qquad s = 1, 2, \ldots , \tag{2.4a}$$

$$f_l(k_{ls} R) = 0 ; \qquad s = 1, 2, \ldots , \tag{2.4b}$$

where k_{ls} is the s-th root of the above equation, so s is the ordinal of the roots.

The kinetic and potential energies associated with SO and LO vibrations are

$$E_p = \frac{1}{2} \sum_{n,i} \int_n \mathrm{d}\boldsymbol{r} \left\{ \frac{\theta_n(\omega_{i,n})}{\varepsilon_0 \omega_{pn}^2} \left[\boldsymbol{p}_n^{i*}(\boldsymbol{r})\, \boldsymbol{p}_n^i(\boldsymbol{r}) + \omega_{i,n}^2 \boldsymbol{p}_n^{i*}(\boldsymbol{r})\, \boldsymbol{p}_n^i(\boldsymbol{r}) \right] \right\} , \tag{2.5}$$

where the symbol "i" denotes the corresponding quantities belonging to the SO or LO vibration. ω_{pn} (the ion plasma frequency of the material n) and θ_n are, respectively

$$\omega_{pn} = \frac{n_n e^2}{\varepsilon_0 \mu_n}, \qquad \theta_n^{1/2} = [1 + n_n \alpha_n (\lambda_{0n} - \lambda_n)]^{-1} \tag{2.6}$$

Here we have used the following abbreviations:

$$\lambda_{0n} = \frac{\mu_n \omega_{0n}^2}{n_n e^2}, \qquad \lambda_n = \frac{\mu_n \omega_{i,n}^2}{n_n e^2}.$$

In all the above expressions, α_n is the electronic polarizability of the material n, n_n the number of the positive and negative ions or Wigner-Seitz cells per unit volume, μ_n their reduced mass, ω_{0n} the characteristic frequency of the ionic vibration.

Thus, the Hamiltonian of the system consisting of a mobile charge carrier (electron or hole) and the polarization modes associated with SO and LO vibrations, can be written as

$$H = -\frac{\hbar^2}{2m^*_{e,h}} \nabla^2_{e,h} + V_{e,h} + \sum_i \sum_{n=1}^{2} \int_n \boldsymbol{D}(\boldsymbol{r} - \boldsymbol{r}_{e,h})\, \boldsymbol{p}_n^i(\boldsymbol{r})\, d\boldsymbol{r} + E_p\,, \tag{2.7}$$

where the subscript e or h refers the electron or hole, $V_{e,h}$ is the potential difference of the electron or hole at the interface of both dielectrics, the third term is the interaction energy of the electron or hole with SO and LO polarization modes in which $\boldsymbol{D}(\boldsymbol{r} - \boldsymbol{r}_{e,h})$ is the electric displacement vector at $\boldsymbol{r}$ caused by the electron or hole at $\boldsymbol{r}_{e,h}$.

Because the motion of the ions is described by classical mechanics, only when the kinetic energy of the ions vanishes and their potential energy has a minimum, the total energy of the system can have a minimum. As pointed out by Pekar [9], corresponding to a definite polarization strength $\boldsymbol{p}$, the potential of the ions is given by

$$\boldsymbol{F}(\psi, \boldsymbol{p}) = -\frac{\hbar^2}{2m^*_{e,h}} \langle \psi(\boldsymbol{r}_{e,h}) | \nabla^2_{e,h} | \psi(\boldsymbol{r}_{e,h}) \rangle - \sum_n \sum_i \int_n \boldsymbol{D}(\psi, \boldsymbol{r})\, \boldsymbol{p}_n^i(\boldsymbol{r})\, d\boldsymbol{r} +$$

$$+ \frac{1}{2} \sum_n \sum_i \int_n d\boldsymbol{r} \left\{ \frac{\theta_n(\omega_{i,n})}{\varepsilon_0 \omega_{pn}^2}\, \omega_{i,n}^2 \boldsymbol{p}_n^{i*}(\boldsymbol{r})\, \boldsymbol{p}_n^i(\boldsymbol{r}) \right\}, \tag{2.8}$$

where

$$\boldsymbol{D}(\psi, \boldsymbol{r}) = \mp \frac{e}{4\pi\varepsilon_0} \langle \psi(\boldsymbol{r}_{e,h}) | \nabla_{\boldsymbol{r}} \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_{e,h}|} | \psi(\boldsymbol{r}_{e,h}) \rangle\,, \tag{2.9}$$

and $\psi(\boldsymbol{r}_{e,h})$ is the wave function of the mobile charge carrier. If we substitute such a wave function $\psi(\boldsymbol{r}_{e,h})$ into (2.8) that $F(\psi, \boldsymbol{r})$ is optimum, this $\psi(\boldsymbol{r}_{e,h})$ is the stationary state of the charge carrier which adiabatically corresponds to the configuration of ions $\boldsymbol{p}$. However, the ions are, in general, not in an equilibrium state. In order to minimize the potential energy of the ions, it is necessary to minimize $F(\psi, \boldsymbol{p})$ with respect to $\boldsymbol{p}$. However, in the situation under consideration, only the $C^{so}_{lm,n}$ and $C^{lo}_{lm,n}$ are adjustable quantities. Thus, the optimization of $F(\psi, \boldsymbol{p})$ with respect to $\boldsymbol{p}$ should be changed to that with respect to $C^{so}_{lm,n}$ and $C^{lo}_{lm,n}$. Consequently these coefficients can be determined. They are

$$C^{so}_{lm,1} = \frac{A_1^{so} + A_2^{so}}{B_1^{so} + B_2^{so}}, \qquad C^{lo}_{lm,n} = \frac{1}{\omega^2_{lo,n}} \frac{\varepsilon_0 \omega_{pn}^2}{\theta_n} \frac{A_n^{lo}}{B_n^{lo}}, \tag{2.10}$$

where

$$A_1^{so} = \int \langle \psi(\boldsymbol{r}_{e,h})| \boldsymbol{D}(\boldsymbol{r} - \boldsymbol{r}_{e,h}) |\psi(\boldsymbol{r}_{e,h})\rangle \, \boldsymbol{p}_{lm,1}^{so}(\boldsymbol{r}) \, d\boldsymbol{r} ,$$

$$A_2^{so} = \left(\frac{x_2}{x_1}\right) \int \langle \psi(\boldsymbol{r}_{e,h})| \boldsymbol{D}(\boldsymbol{r} - \boldsymbol{r}_{e,h}) |\psi(\boldsymbol{r}_{e,h})\rangle \, \boldsymbol{p}_{lm,2}^{so}(\boldsymbol{r}) \, d\boldsymbol{r} ,$$

$$B_1^{so} = \left(\frac{\theta_1}{\varepsilon_0 \omega_{p1}^2}\right) \omega_{so,1}^2 \int_1 |\boldsymbol{p}_{lm,1}^{so}(\boldsymbol{r})|^2 \, d\boldsymbol{r} ,$$

$$B_2^{so} = \left(\frac{x_2}{x_1}\right)^2 \left(\frac{\theta_2}{\varepsilon_0 \omega_{p2}^2}\right) \omega_{so,2}^2 \int_2 |\boldsymbol{p}_{lm,2}^{so}(\boldsymbol{r})|^2 \, d\boldsymbol{r} , \tag{2.11}$$

$$A_n^{lo} = \int_n \langle \psi(\boldsymbol{r}_{e,h})| \boldsymbol{D}(\boldsymbol{r} - \boldsymbol{r}_{e,h}) |\psi(\boldsymbol{r}_{e,h})\rangle \, \boldsymbol{p}_{lm,n}^{lo}(\boldsymbol{r}) \, d\boldsymbol{r} ,$$

$$B_n^{lo} = \int_n |\boldsymbol{p}_{lm,n}^{lo}(\boldsymbol{r})|^2 \, d\boldsymbol{r} .$$

From the results obtained above the energy of the charge carrier can be determined which is given by

$$E^{e,h} = -\frac{\hbar^2}{2m_{e,h}^*} \langle \psi(\boldsymbol{r}_{e,h})| \nabla^2 - \frac{2m_{e,h}^*}{\hbar^2} V_{e,h} |\psi(\boldsymbol{r}_{e,h})\rangle -$$

$$- \sum_n \sum_i \int_n \psi(\boldsymbol{r}_{e,h}) \, | \boldsymbol{D}(\boldsymbol{r} - \boldsymbol{r}_{e,h}) |\psi(\boldsymbol{r}_{e,h})\rangle \, \boldsymbol{p}_n^i(\boldsymbol{r}) \, d\boldsymbol{r} .$$

Substituting $C_{lm,1}^{so}$ and $C_{lm,n}^{lo}$ into the above expression gives

$$E^{e,h} = -\frac{\hbar^2}{2m_{e,h}^*} \langle \psi(\boldsymbol{r}_{e,h})| \nabla_{e,h}^2 - \frac{2m_{e,h}^*}{\hbar^2} V_{e,h} |\psi(\boldsymbol{r}_{e,h})\rangle -$$

$$- \sum_{lm} \frac{[A_1^{so} + A_2^{so}]^2}{B_1^{so} + B_2^{so}} - \sum_{n=1}^{2} \sum_{lm} \frac{\varepsilon_0 \omega_{pn}^2}{\theta_n \omega_{lo,n}^2} \frac{[A_n^{lo}]^2}{B_n^{lo}} , \tag{2.12}$$

where the second and the last terms are the interaction energy of the charge carrier with SO and LO vibrations, respectively. Now, we turn to discuss two such terms still further.

2.1 The interaction energy of the charge carrier with SO vibrations

According to (2.12), the calculation of the interaction energy of the charge carrier with SO vibrations is to evaluate $(A_1^{so} + A_2^{so})$ and $(B_1^{so} + B_2^{so})$. For $(A_1^{so} + A_2^{so})$, we have from (2.11)

$$A_1^{so} + A_2^{so} = -\frac{e}{4\pi\varepsilon_0} \langle \psi(\boldsymbol{r}_{e,h})| \left\{ \int_1 \nabla_{\boldsymbol{r}} \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_{e,h}|} \boldsymbol{p}_{lm,1}^{so}(\boldsymbol{r}) \, d\boldsymbol{r} + \right.$$

$$\left. + \left(\frac{x_2}{x_1}\right) \int_2 \nabla_{\boldsymbol{r}} \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_{e,h}|} \boldsymbol{p}_{lm,2}^{so}(\boldsymbol{r}) \, d\boldsymbol{r} \right\} |\psi(\boldsymbol{r}_{e,h})\rangle =$$

$$= -\frac{e}{4\pi\varepsilon_0} \langle \psi(\boldsymbol{r}_{e,h}) | \left\{ \int_1 \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_{e,h}|} \nabla_r \boldsymbol{p}^{so}_{lm,1}(\boldsymbol{r})\, d\boldsymbol{r} - \right.$$

$$\left. - \int_{s_1} \frac{1}{|\boldsymbol{R} - \boldsymbol{r}_{e,h}|} \boldsymbol{N}_1 \boldsymbol{p}^{so}_{lm,1}(\boldsymbol{R})\, ds_R \right\} |\psi(\boldsymbol{r}_{e,h})\rangle -$$

$$- \frac{e}{4\pi\varepsilon_0} \left(\frac{x_2}{x_1}\right) \langle \psi(\boldsymbol{r}_{e,h}) | \left\{ \int_2 \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_{e,h}|} \nabla_r \boldsymbol{p}^{so}_{lm,2}(\boldsymbol{r})\, d\boldsymbol{r} + \right.$$

$$\left. + \int_{s_2} \frac{1}{|\boldsymbol{R} - \boldsymbol{r}_{e,h}|} \boldsymbol{N}_1 \boldsymbol{p}^{so}_{lm,2}(\boldsymbol{R})\, ds_R \right\} |\psi(\boldsymbol{r}_{e,h})\rangle ,$$

where $\boldsymbol{N}_1$ is the unit normal vector on the interface. Because of $\nabla \boldsymbol{p}^{so}_{lm,n} = 0$, the above expression is simplified to

$$A_1^{so} + A_2^{so} =$$

$$= \frac{e}{4\pi\varepsilon_0} \langle \psi(\boldsymbol{r}_{e,h}) | \int_s \frac{1}{|\boldsymbol{R} - \boldsymbol{r}_{e,h}|} \left[l + (l+1) \frac{x_2}{x_1} \right] \frac{1}{R^2}\, Y_l^m(\hat{R})\, ds_R\, |\psi(\boldsymbol{r}_{e,h})\rangle =$$

$$= \frac{e}{4\pi\varepsilon_0} \langle \psi(\boldsymbol{r}_{e,h}) | \int_s \sum_{l'} \frac{r^{l'}_{e,h}}{R^{l'+1}}\, p_{l'}(u) \left[l + (l+1) \frac{x_2}{x_1} \right] \frac{1}{R^2}\, Y^m(R)\, ds_R\, |\psi(\boldsymbol{r}_{e,h})\rangle ,$$

where $p_l(u)$ is the Legendre polynomial, u the cosine of the angle between $\boldsymbol{R}$ and $\boldsymbol{r}_{e,h}$:

$$p_l(u) = \frac{4\pi}{2l+1}\, Y_l^{m*}(\hat{R})\, Y_l^m(\hat{r}_{e,h}) .$$

Thus, $(A_1^{so} + A_2^{so})$ is immediately changed to

$$A_1^{so} + A_2^{so} = \frac{e}{\varepsilon_0} \langle \psi(\boldsymbol{r}_{e,h}) | \frac{1}{2l+1} \left[l + (l+1) \frac{x_2}{x_1} \right] \frac{r^l_{e,h}}{R^{l+1}}\, Y_l^m(\hat{r}_{e,h})\, |\psi(\boldsymbol{r}_{e,h})\rangle . \tag{2.13}$$

As for $(B_1^{so} + B_2^{so})$, the calculation is easy. The result is

$$B_1^{so} + B_2^{so} = \left(\frac{\theta_1 \omega^2_{so,1}}{\varepsilon_0 \omega^2_{p1}}\right) l^2 \int_0^R \frac{r^{2l}}{R^{2(l+1)}}\, dr + \left(\frac{\theta_2 \omega^2_{so,2}}{\varepsilon_0 \omega^2_{p2}}\right) \left[(l+1) \frac{x_2}{x_1} \right]^2 \int_R \frac{R^{2l}}{r^{2(l+1)}}\, dr =$$

$$= \frac{\omega^2_{so}}{\varepsilon_0} \frac{1}{2(l+1)R} \left\{ l^2 \frac{\theta_1}{\omega^2_{p1}} + \left[(l+1) \frac{x_2}{x_1} \right]^2 \frac{\theta_2}{\omega^2_{p2}} \right\}. \tag{2.14}$$

Here it is considered that the SO vibration has the same frequency. Inserting the above results (2.13) and (2.14) into the second term of (2.12), then the interaction energy of the charge carrier with SO vibrations (denoted by E^{so}_{ep}) is finally expressed as

$$E^{so}_{ep} = -\left(\frac{e^2}{\varepsilon_0}\right) \frac{\{ \langle \psi(\boldsymbol{r}_{e,h}) | \left[l + (l+1)\, (x_2/x_1) \right] R^{-(l+1)} r^l_{e,h} Y_l^m(\hat{r}_{e,h})\, |\psi(\boldsymbol{r})_{e,h}\rangle \}^2}{2(l+1)\, \omega^2_{so} R [l^2(\theta_1/\omega^2_{p1}) + (l+1)^2\, (x_2/x_1)^2\, (\theta_2/\omega^2_{p2})]} . \tag{2.15}$$

2.2 *The interaction energy of the charge carrier with LO vibration*

The last term of (2.12) is the interaction energy of the charge carrier with LO vibrations. Assume the charge carrier to be in the inner spherical dielectric 1, and its wave function to be represented by $\psi_1(\boldsymbol{r}_{e,h})$. Then, from (2.11) A_1^{lo} can be written as

$$
\begin{aligned}
A_1^{lo} = & -\frac{e}{4\pi\varepsilon_0}\langle\psi(\boldsymbol{r}_{e,h})|\int_1 \nabla_r \frac{1}{|\boldsymbol{r}-\boldsymbol{r}_{e,h}|}\,\boldsymbol{p}^{lo}_{lm,1}\,\mathrm{d}\boldsymbol{r} + \\
& + \int_2 \nabla_r \frac{1}{|\boldsymbol{r}-\boldsymbol{r}_{e,h}|}\,\boldsymbol{p}^{lo}_{lm,2}\,\mathrm{d}\boldsymbol{r}\,|\psi(\boldsymbol{r}_{e,h})\rangle = \\
= & -\frac{e}{4\pi\varepsilon_0}\langle\psi(\boldsymbol{r}_{e,h})|\int_1 \frac{1}{|\boldsymbol{r}-\boldsymbol{r}_{e,h}|}\,\nabla_r\,\boldsymbol{p}^{lo}_{lm,1}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} - \\
& - \int_{s_1} \frac{1}{|\boldsymbol{R}-\boldsymbol{r}_{e,h}|}\,\boldsymbol{N}_1\boldsymbol{p}^{lo}_{lm,1}(\hat{R})\,\mathrm{d}s_R\,|\psi(\boldsymbol{r}_{e,h})\rangle - \\
& - \frac{e}{4\pi\varepsilon_0}\langle\psi_1(\boldsymbol{r}_{e,h})|\int_2 \frac{1}{|\boldsymbol{r}-\boldsymbol{r}_{e,h}|}\,\nabla_r\boldsymbol{p}^{lo}_{lm,2}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} + \\
& + \int_{s_2} \frac{1}{|\boldsymbol{R}-\boldsymbol{r}_{e,h}|}\,\boldsymbol{N}_1\boldsymbol{p}^{lo}_{lm,2}(\hat{R})\,\mathrm{d}s_R\,|\psi_1(\boldsymbol{r}_{e,h})\rangle = \\
= & -\frac{e}{4\pi\varepsilon_0}\langle\psi_1(\boldsymbol{r}_{e,h})|\left\{\int_0^{r_{e,h}}\int_\Omega \sum_l (r^l/r_{e,h}^{l+1})\,p_l(\hat{r}\cdot\hat{r}_{e,h})\nabla^2[j_{l'}(k_{l'}r)\,Y_{l'}^{m'}(\hat{r})]\,\mathrm{d}r\,\mathrm{d}\Omega + \right. \\
& + \int_{r_{e,h}}^{R}\int_\Omega \sum_l (r_{e,h}^l/r^{l-1})\,p_l(\hat{r}\cdot\hat{r}_{e,h})\,\nabla^2[j_{l'}(k_{l'}r)\,Y_{l'}^{m'}(\hat{r})]\,\mathrm{d}r\,\mathrm{d}\Omega - \\
& \left. - \int_\Omega \sum (r_{e,h}^l/R^{l-1})\,p_l(\hat{R}\cdot\hat{r}_{e,h})\left[\frac{\partial}{\partial r}\,j_{l'}(k_{l'}r)\right]_R Y_{l'}^{m'}(\hat{R})\,\mathrm{d}\Omega\right\}|\psi(\boldsymbol{r}_{e,h})\rangle - \\
& - \frac{e}{4\pi\varepsilon_0}\langle\psi_1(\boldsymbol{r}_{e,h})|\left\{\int_R\int_\Omega \sum_l (r_{e,h}^l/r^{l-1})\,p_l(\hat{r}\cdot\hat{r}_{e,h})\nabla^2[f_{l'}(k_{l'}r)\,Y_{l'}^{m'}(\hat{r})]\,\mathrm{d}r\,\mathrm{d}\Omega - \right. \\
& \left. - \int_\Omega \sum_l (r_{e,h}^l/R^{l-1})\,p_l(\hat{R}\cdot\hat{r}_{e,h})\left[\frac{\partial}{\partial r}\,f_{l'}(k_{l'}r)\right]_R Y_{l'}^{m'}(\hat{R})\,\mathrm{d}\Omega\right\}|\psi_1(\boldsymbol{r}_{eh})\rangle\ .
\end{aligned}
$$

In the above expression the second term comes from the interaction of the charge carrier in the dielectric 1 with LO vibrations in dielectric 2. This term vanishes from the boundary condition $f_l(k_lR) = 0$. Thus, only the first term coming from the interaction of the charge carrier with LO vibrations in dielectric 1 is left. After some simple calculations, it gives

$$
A_1^{lo} = \frac{e}{\varepsilon_0}\langle\psi(\boldsymbol{r}_{e,h})|\,j_l(k_{ls}r)\,Y_l^m(\hat{r}_{e,h})\,|\psi(\boldsymbol{r}_{e,h})\rangle\ , \tag{2.16}
$$

where the subscript "s" is the ordinal of the roots k_{ls} which is obtained from the boundary condition $j_l(k_l R) = 0$.

As for B_1^{lo}, the calculation is straightforward. The result is

$$B_1^{\mathrm{lo}} = \int_1 |p_{lm,1}^{\mathrm{lo}}(\boldsymbol{r})|^2 \, \mathrm{d}\boldsymbol{r} = k_{ls}^2 \int_0^R j_l^2(k_{ls} r) \, r^2 \, \mathrm{d}r = (\pi/4) \, k_{ls} R^2 [J_{l+3/2}(k_{ls} r)]^2 \,, \quad (2.17)$$

where $J_{l+3/2}$ is the Bessel function of the second kind. Thus, the interaction energy of the charge carrier in dielectric 1 with LO vibrations is finally written as (denoted by $E_{\mathrm{ep},1}^{\mathrm{lo}}$)

$$E_{\mathrm{ep},1}^{\mathrm{lo}} = -\frac{e^2}{\varepsilon_0} \sum_{lm} \sum_{s} \frac{\omega_{p1}^2}{\theta_1 \omega_{\mathrm{lo},1}^2} \frac{\{\langle \psi_1(\boldsymbol{r}_{\mathrm{e,h}}) | \; j_l(k_{ls} r)) \; Y_l^m(\hat{r}_{\mathrm{e,h}}) \, | \psi_1(\boldsymbol{r}_{\mathrm{e,h}}) \rangle \}^2}{(\pi/4) \, k_{ls} R^2 [J_{l+3/2}(k_{ls} R)]^2} \,. \quad (2.18)$$

Analogously, one can also prove that the charged particle in dielectric 2 interacts only with LO vibrations in dielectric 2. The interaction energy is

$$E_{\mathrm{ep},2}^{\mathrm{lo}} = -\frac{e^2}{\varepsilon_0} \sum_{lm} \sum_{s} \frac{\omega_{p2}^2}{\theta_2 \omega_{\mathrm{lo},2}^2} \frac{\{\langle \psi_2(\boldsymbol{r}_{\mathrm{e,h}}) | \; f_l(k_{ls} r) Y_l^m(\hat{r}_{\mathrm{e,h}}) \, | \psi_2(\boldsymbol{r}_{\mathrm{e,h}}) \rangle \}^2}{k_{ls}^2 \int_R |f_l(k_{ls} r)|^2 \, r^2 \, \mathrm{d}r} \,. \quad (2.19)$$

Here we would like to point out from the above results (2.18) and (2.19) that the charge carrier in the inner dielectric spheroid only interacts with LO vibrations of this inner spheroid, it does not interact with LO vibrations of outer dielectric spherical layers, and vice verse. This fact is important. Because the potential difference between both dielectrics is not infinite, the carriers have a definite probability to enter from one dielectric into the other by the tunnel effect. In this case, the interaction of the carrier with LO vibrations in various layers can be separately taken into consideration. This is why the wave functions in (2.18) and (2.19) are expressed in terms of ψ_1 and ψ_2, respectively.

Finally, inserting these results (2.15), (2.18), and (2.19) into (2.12) gives the total energy of the charge carrier to be

$$\begin{aligned} E^{\mathrm{e,h}} = & -\frac{\hbar^2}{2m_{\mathrm{e,h}}^*} \langle \psi(\boldsymbol{r}_{\mathrm{e,h}}) | \; \nabla_{\mathrm{e,h}}^2 - \frac{2m_{\mathrm{e,h}}^*}{\hbar^2} \, V_{\mathrm{e,h}} \, | \psi(\boldsymbol{r}_{\mathrm{e,h}}) \rangle - \\ & - \frac{e^2}{\varepsilon_0} \sum_{lm} \frac{\{\langle \psi(\boldsymbol{r}_{\mathrm{e,h}}) | \; [l + (l+1) \, (x_2/x_1)] \; R^{-(l+1)} r_{\mathrm{e,h}}^l Y_l^m(\hat{r}_{\mathrm{e,h}}) \, | \psi(\boldsymbol{r}_{\mathrm{eh}}) \rangle \}^2}{(2l+1) \, \omega_{\mathrm{so}}^2 R[l^2(\theta_1/\omega_{p1}^2) + (l+1)^2 \, (x_2/x_1)^2 \, (\theta_2/\omega_{p2}^2)]} - \\ & - \frac{e^2}{\varepsilon_0} \sum_{lm} \sum_{s} \frac{\omega_{p1}^2}{\theta_1 \omega_{\mathrm{lo},1}^2} \frac{\{\langle \psi_1(\boldsymbol{r}_{\mathrm{e,h}}) | \; j_l(k_{ls} r_{\mathrm{e,h}}) \; Y_l^m(\hat{r}_{\mathrm{e,h}}) \, | \psi_1(\boldsymbol{r}_{\mathrm{e,h}}) \rangle \}^2}{(\pi/4) \, k_{ls}^2 [J_{l+3/2}(k_{ls} R)]^2} - \\ & - \frac{e^2}{\varepsilon_0} \sum_{lm} \sum_{s} \frac{\omega_{p2}^2}{\theta_2 \omega_{\mathrm{lo},2}^2} \frac{\{\langle \psi_2) \boldsymbol{r}_{\mathrm{e,h}}) | \; f_l(k_{ls} r_{\mathrm{e,h}}) \; Y_l^m(\hat{r}_{\mathrm{e,h}}) \, | \psi_2(\boldsymbol{r}_{\mathrm{e,h}}) \rangle \}^2}{k_{ls}^2 \int_R |f_l(k_{ls} r)|^2 \, r^2 \, \mathrm{d}r} \,. \end{aligned} \quad (2.20)$$

The above expression is derived for dielectric 1 to be embedded in another polar crystal. If the dielectric 2 is another non-polar material, how will the above result be changed? In this case, the field energy $(\varepsilon_0 \varepsilon_{22}/2) \int_2 E_2^2 \, \mathrm{d}\tau$ should be used instead of $(\theta_2 \omega_{\mathrm{lo},2}^2/\varepsilon_0 \omega_{p2}^2) \times$ $\times \int_2 |p_2^{\mathrm{lo}}|^2 \, \mathrm{d}\tau$. Since there is a relation between the electric field and the polarization vector $\boldsymbol{E}_2 = (\varepsilon_0 \, x_2)^{-1} \, \boldsymbol{p}_2$,

$$(\varepsilon_0 \varepsilon_2/2) \int E_2^2 \, \mathrm{d}\tau = (\varepsilon_2/2\varepsilon_0 x_2) \int_2 p_2^2 \, \mathrm{d}\tau \,. \quad (2.21)$$

Here ε_2 and x_2 are the real dielectric constant and susceptibility instead of the dielectric function of the previous case. Then, the energy of the charge carrier for the case of the microcrystallite being embedded in a non-polar material may be immediately written down. It is

$$E^{e,h} = -\frac{\hbar^2}{2m^*_{e,h}} \left\langle \psi(\boldsymbol{r}_{e,h}) | \nabla_{e,h} - \frac{2m^*_{e,h}}{\hbar^2} V_{e,h} | \psi(\boldsymbol{r}_{e,h}) \right\rangle - \\ -\frac{e^2}{\varepsilon_0} \sum_{lm} \frac{\{\langle \psi(\boldsymbol{r}_{e,h}) | [l+(l+1)(x_2/x_1)] R^{-(l+1)} r^l_{e,h} Y^m_l(\hat{r}_{e,h}) | \psi(\boldsymbol{r}_{e,h}) \rangle\}^2}{(2l+1) R[l^2(\theta_1 \omega^2_{so}/\omega^2_{p1}) + (l+1)^2 \varepsilon_2 x_1^{-1}]} - \\ -\frac{e^2}{\varepsilon_0} \sum_{lm} \sum_{s} \frac{\omega^2_{p1}}{\theta_1 \omega^2_{lo,1}} \frac{\{\langle \psi_1(\boldsymbol{r}_{e,h}) | j_l(k_{ls} k_{e,h}) Y^m_l(\hat{r}_{e,h}) | \psi_1(\boldsymbol{r}_{e,h}) \rangle\}^2}{(\pi/4) k^2_{ls} [J_{l+3/2}(k_{ls} R)]^2}. \quad (2.22)$$

In this expression such as the last term of (2.20) disappears. This is because in a non-polar material there is only one kind of polarization mode characterized by (2.1b). The interaction of the carrier with this polarization mode has been contained in the second term of the above expression.

3. Calculations and Conclusions

In what follows, we turn to calculate the energy of the charge carrier by making use of (2.20) or (2.22) for the infinitely and finitely deep potential well, respectively. Assume the charge carrier to be an electron.

3.1 The case of the infinitely deep potential well

By the infinitely deep potential well it is meant

$$V_e = 0; \qquad r < R,$$
$$V_e = \infty; \qquad r > R.$$

In this case the electron is completely localized in the inner dielectric spheroid. Then, the last term of (2.20) disappears. When the interaction of the electron with SO and LO vibrations is not taken into consideration, as one knows, the ground state wave function $\psi(\boldsymbol{r})$ can be exactly obtained from the Schrödinger equation

$$\frac{\hbar^2}{2m^*_e} \nabla^2_e \psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}),$$

which gives

$$\psi(\boldsymbol{r}) = A \frac{1}{r} \sin\left(\frac{\pi}{R} r\right), \quad (3.1)$$

where A is the normalization coefficient. If the interaction of the electron with SO and LO vibrations is taken into consideration, according to Pekar's idea, the wave function of the electron should be determined from the optimal condition of the function $F(\psi, \boldsymbol{p})$ with respect to some chosen trial function containing one or more variational parameters. However, for the present problem, because the microcrystallite is very small, the term of the kinetic energy will play the principal role for the wave function in compairson with the interaction energy. Thus, the interaction term can be regarded as a perturbation, and (3.1) as the zero-order approximate wave function. It is expected that the energy obtained by such a perturbation method is, at least, not worse than by the variational one. Because this approximate wave function chosen by

the above consideration does not contain a factor such as the spherical harmonics Y_l^m, l and m in the energy expression (2.20) must be zero. Then, inserting the zero-order approximate function (3.1) into (2.20), gives $E_{ep}^{so} = 0$ and

$$E^e = \frac{\hbar^2\pi^{22}}{2m_e^* R^2} - \frac{e^2}{\varepsilon_0}\sum_s \frac{\omega_{p1}^2}{\theta_1\omega_{L,1}^2}\frac{\{\langle\psi|\, j_0(k_{0s}r)\,|\psi\rangle\}^2}{(\pi/4)\, k_{0s}R^2 J_{3/2}^2(k_{0s}R)} \,. \tag{3.2}$$

It means that the electron does not interact with SO vibrations for the first-order approximate energy. Because of

$$(\omega_{pn}^2/\theta_n) = \omega_{L,n}^2[(1/\varepsilon_{\infty n}) - (1/\varepsilon_{sn})] \,. \tag{3.3}$$

where $\varepsilon_{\infty n}$ and ε_{sn} are the high-frequency and static dielectric constant of the layer n, respectively, after some calculations the above expression becomes

$$E^e = \frac{\hbar^2\pi^2}{2m_e^* R^2} - \frac{e^2}{8\pi^3\varepsilon_0 R}\left(\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{s1}}\right)\sum_s \frac{1}{s^2}\left\{\left(2\int_0^{s\pi} - \int_0^{(s-2)\pi} - \int_0^{(s+2)\pi}\right)\frac{\sin r}{r}\,dr\right\}^2 .$$

Using $E_0 = (\hbar^2/2m^*a_0^2)$ as energy unit, $a_0 = (4\pi\varepsilon_0\hbar^2/m_e^* e^2)$ as the length unit, i.e. put $\bar{E}^e = (E^e/E_0)$, $x = (R/a_0)$, the above result gives

$$\bar{E}^e = \frac{\pi^2}{x^2} - \frac{1}{x}\left(\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{s1}}\right)\sum_s \frac{1}{s^2}\left\{\left[2\int_0^{s\pi} - \int_0^{(s-2)\pi} - \int_0^{(s+2)\pi}\right]\frac{\sin r}{r}\,dr\right\}^2 . \tag{3.4}$$

The curves 1 in Fig. 1 and 2 are, respectively, the calculated results by using the above expression for CdS and CuCl microcrystallites under the assumption of an infinitely deep potential well, curve 1′ in Fig. 1 is that without containing the interaction of the electron with LO vibrations. One can see from both the curves 1 and 1′ that the interaction energies are about a tenth of the total energy at various x values.

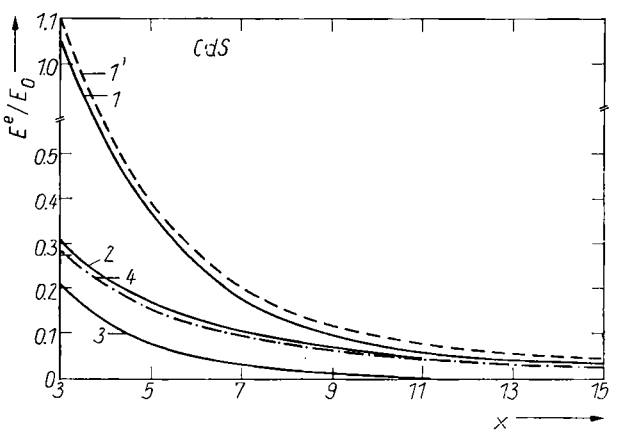

Fig. 1. The ground state energy of an electron in CdS ($m_1^* = 0.19m_0$) crystallites as a function of the crystallite radius x ($= R/a_0$). Curves (1) to (4): the interaction energy between the electron and LO vibrations is taken into account (except curve 1′). (1) and (1′): for the infinitely deep potential well; (2) finitely deep potential well, embedded in the air, $V_0 = 4.4$ eV; (3) finitely deep potential well, embedded in NaCl, $V_0 = 3.9$ eV; (4) the same as curve 2, but $V_0 = 3.0$ eV. $E_0 = (\hbar/m_e^* a_0^2) = 2.582$ eV, $a_0 = (4\pi\varepsilon_0\hbar/m^* e^2) = 2.789 \times 10^{-10}$ m

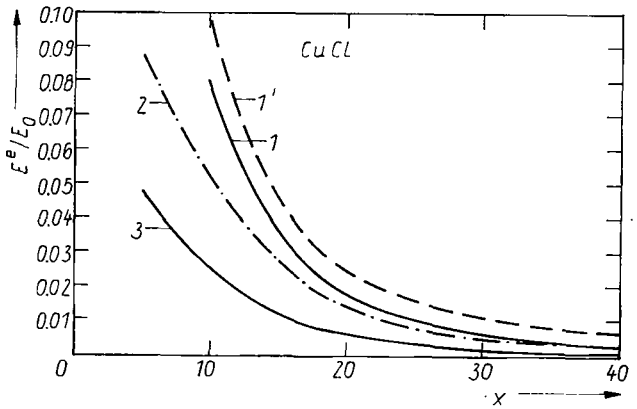

Fig. 2. The ground state energy of an electron in CuCl crystallites ($m_1^* = 0.5m_0$) as a function of the crystallite radius. (1) to (3): the interaction energy between the electron and LO vibrations is taken into account (except curve 1'). (1) and (1'): for infinitely deep potential well; (2) finitely deep potential well, embedded in the air, $V_0 = 3.0$ eV; (3) finitely deep potential well, embedded in NaCl, $V_0 = 2.5$ eV. $E_0 = 6.794$ eV, $a_0 = 1.06 \times 10^{-10}$ m

3.2 The case of the finitely deep potential well

By the finitely deep potential well it is meant

$$V_e = 0; \qquad r < R,$$
$$V_e = V_0; \qquad r > R.$$

V_0 is the potential difference between the inner dielectric spheroid and the outer dielectric spherical layer. In this case, the electron in the inner spheroid has a definite probability to enter into the outer dielectric layer. If the interaction of the electron with SO and LO vibrations is not taken into account, the wave functions of the electron are, respectively,

$$\psi_1(r) = A_1 \frac{1}{r} \sin(kr); \qquad r < R, \tag{3.5a}$$

$$\psi_2(r) = A_2 \frac{1}{r} \exp(-qr); \qquad r > R, \tag{3.5b}$$

where

$$k^2 = (2m_{e,1}^*/\hbar^2)\, E, \qquad q^2 = (2m_{e,2}^*/\hbar^2)\, V_0(1 - E/V_0),$$

A_1 and A_2 are the normalization coefficients which are given by

$$A_1 = \left[2\pi R - \pi \frac{\sin 2kR}{k} + 2\pi \frac{\sin^2 kR}{q}\right]^{-1/2}, \tag{3.6a}$$

$$A_2 = \exp(qR) \sin kR \left[2\pi R - \pi \frac{\sin 2kR}{k} + 2\pi \frac{\sin^2 kR}{q}\right]^{-1/2} \tag{3.6b}$$

The wave functions should also satisfy, at the boundary $r = R$,

$$\psi_1(R) = \psi_2(R), \qquad \frac{1}{m_{e,1}^*} \frac{\partial}{\partial r} \psi_1(r)|_R = \frac{1}{m_{e,2}^*} \frac{\partial}{\partial r} \psi_2(r)|_R. \tag{3.7}$$

The latter is equivalent to the continuity condition for the first-order derivative of the wave functions at the boundary. From these two equations we have

$$\tan kR = kR\left[1 - \frac{m^*_{e,1}}{m^*_{e,2}}(1 + qR)\right]^{-1}. \tag{3.8}$$

Introducing ξ such as to make

$$x_0\xi = kR\,, \qquad x_0 = (2m^*_{e,2}V_0)^{1/2}\,\hbar^{-1}R\,,$$

(3.8) is immediately rewritten as

$$\tan(x_0\xi) = x_0\xi\left[1 - d - x_0 d\left(1 - \frac{\xi^2}{d}\right)\right]^{-1}, \tag{3.9}$$

where $d = (m^*_{e,1}/m^*_{e,2})$. It is evident from this equation that there have a series of ξ_n satisfying this equation. Consequently a series of energies E_n can be determined from ξ_n. If ξ corresponding to the lowest energy state is expressed as ξ_0, the energy of the lowest state is

$$E = \frac{x_0^2\xi_0^2}{2m^*_{e,1}R^2}\,. \tag{3.10}$$

Analogous to the case of Section 3.1, after taking into consideration the interaction of the electron with SO and LO vibrations, the functions (3.5 a) and (3.5 b) can be taken as the zero-order approximations for calculating the energy. Inserting these functions into the energy expression (2.21), one can see that l and m have to be taken zero because the wave functions do not contain a factor such as the spherical harmonics Y_l^m. Consequently (2.21) is simplified to

$$E^e = \frac{x_0^2\xi_0^2}{2m^*_{e,1}R^2} - \frac{e^2}{\varepsilon_0}\sum_s \frac{\omega_{p1}^2}{\theta_1\omega_{L,1}^2}\,\frac{\{\langle\psi_1|\, j_0(k_{0s}r)\,|\psi_1\rangle\}^2}{(\pi/4)\,k_{0s}R^2J_{3/2}^2(k_{0s}R)} - \\ - \frac{e^2}{\varepsilon_0}\sum_s \frac{\omega_{2p}^2}{\theta_2\omega_{L,2}^2}\,\frac{\{\langle\psi_2|\, f_0(k_{0s}r)\,|\psi_2\rangle\}^2}{k_{0s}^2\int |f_0(k_{0s}r)|^2\, r^2\,\mathrm{d}r}\,, \tag{3.11}$$

in which the interaction term of the electron with SO vibrations disappears. The second term in the above expression is similar to the corresponding term in the previous Section 3.1. Thus, the result can be easily obtained by repeating the calculation procedures of the previous section. The last term is the interaction energy of the electron with LO vibrations in the outer spherical dielectric layer. For calculating this term, we have to assume that the inner and outer radii of the outer spherical layer are, respectively, R_1 and R_2. Then, from the boundary condition $f_0(k_{0s}R_1) = f_0(k_{0s}R_2) = 0$ we have

$$j_0(k_{0s}R_1)\,n_0(k_{0s}R_2) = j_0(k_{0s}R_2)\,n_0(k_{0s}R_1)\,,$$

which gives

$$k_{0s}(R_2 - R_1) = s\pi; \qquad s = 1, 2, \ldots \tag{3.12}$$

Making use of this condition, the calculation of the last term in (3.11) is straightforward. The final result is

$$\frac{e^2}{\varepsilon_0}\sum_s \frac{\omega_{p2}^2}{\theta_2\omega_{L,2}^2}\,\frac{8A_2^4\exp(-4qR)}{sk_{0s}}\int_{R_1}^{R_2}\exp[-2q(r - R_1)]\sin[k_{0s}(r - R_1)]\,\frac{1}{r}\,\mathrm{d}r$$

$$= \frac{e^2}{\varepsilon_0}\sum_s \frac{\omega_{p2}^2}{\theta_2\omega_{L,2}^2}\,\frac{2\sin^4 kR}{2^2\pi^3R_1}\left(\frac{R_2}{R_1} - 1\right)\left(1 - \frac{\sin 2kR_1}{2kR_1} + \frac{\sin^2 kR_1}{qR_1}\right)^{-2} \times$$

$$\times\left[\int_1^2 \exp\left[-2\left(\frac{R_2}{R_1} - 1\right)qR_1(y - 1)\right]\left(\frac{\sin s\pi(y - 1)}{y}\,\mathrm{d}y\right]^2. \tag{3.13}$$

It seems that this result intensively depends on the values of (R_2/R_1). However, it is found by careful investigation that when the values of (R_2/R_1) are taken 2 and 10, the difference of the calculated results is within the required precision. Thus, it can be simply taken as 2.

According to the above discussions and calculations, the energy of the electron is finally expressed as

$$\bar{E}^{e} = \frac{(x_0\xi_0)^2}{x^2} - \frac{1}{x}\left(\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{s1}}\right)\frac{1}{\pi^2}\sum_s \frac{1}{s^2}\left(1 - \frac{\sin 2kR}{2kR} + \frac{\sin^2 kR}{qR}\right)^{-2} \times$$
$$\times \left\{\left[2\int_0^{s\pi} - \int_0^{s\pi - 2x_0\xi_0} - \int_0^{s\pi + 2x_0\xi_0}\right]\frac{\sin r}{r}\,\mathrm{d}r\right\}^2 -$$
$$- \frac{1}{x}\left(\frac{1}{\varepsilon_{\infty 2}} - \frac{1}{\varepsilon_{s2}}\right)\frac{16}{\pi^2}\sum_s \frac{1}{s^2}\sin^4 kR\left(1 - \frac{\sin 2kR}{2kR} + \frac{\sin^2 kR}{qR}\right)^{-2} \times$$
$$\times \left\{\int_1^2 \exp\left[-2qR(y-1)\right]\frac{\sin s\pi(y-1)}{y}\,\mathrm{d}y\right\}^2 . \qquad (3.14)$$

This expression is derived for the microcrystallite embedded in another spherical polar crystal. If the crystallite is embedded in a non-polar material, for example, in air, the last term in the above expression should be given up. The curves 2 and 3 in Fig. 1 and 2 are the results calculated from the above expression for CdS and CuCl crystallites embedded in air and NaCl crystal, respectively. In order to illustrate the influence of V_0 on the energy of the electron, we have also calculated the energy for the CdS crystallite embedded in air, but $V_0 = 3.0$ eV is assumed instead of $V_0 = 4.4$ eV, the calculated results are illustrated by curve 4 in Fig. 1. It shows that the energy of the electron will decrease with the value of V_0. In the calculations of the energy, the values of s are taken from 1 to 5. The various parameters used in the calculation are given in Table 1.

Table 1

The values of parameters used in the calculation

dielectric 1	embedded in medium 2	CdS/air	CdS/NaCl	CuCl/air	CuCl/NaCl
$\varepsilon_{\infty 1}$		5.27	5.27	5.1	5.1
ε_{s1}		8.42	8.42	9.8	9.8
	$\varepsilon_{\infty 2}$	1	2.3	1	2.3
	ε_{s2}		5.8		5.8
$m_1^*(m_0)$		0.19	0.19	0.5	0.5
	$m_2^*(m_0)$	1	2.78	1	2.78
V_0(eV)		4.4; 3.0	3.9	3.0	2.5

3.3 Some conclusions

For the crystallites embedded in another polar or non-polar material, the charge carrier in such a crystallite will rapidly increase with decreasing size of the crystallite. It is verified that the charged particle interacts only with the LO vibrations of the dielectric in which the charged particle is located, and in first-order approximation in the energy the charged particle does not interact with SO vibrations.

All the calculations of the present paper are derived in the long-wave approximation for the lattice vibrations. If the size of the crystallite is decreased to rather small values, the long-wave approximation is no longer suitable, and the irregularities on the surface of the crystallites are also serious. Thus, the present theoretical consideration is not suitable to rather small crystallites. If we take the diameter of the crystallite larger than $a_0 = (4\pi\varepsilon_0\varepsilon\hbar^2/m^*e^2)$ as the criterion for the long-wave approximation to be applicable, the value of $x = (R/a_0)$ for CdS and CuCl crystallites is required, at least, to be larger than 5.

Finally, we would like to point out that the present theoretical considerations are also suitable for the calculation of the ionization and affinity potentials for a charged particle in a crystallite. This problem is important for the chemical and catalytic surface reactions in which crystallites take part.

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