

Effective mass of the surface polaron at a finite temperature

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1994 J. Phys.: Condens. Matter 6 8167

(<http://iopscience.iop.org/0953-8984/6/40/008>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.151

The article was downloaded on 12/05/2010 at 20:41

Please note that [terms and conditions apply](#).

Effective mass of the surface polaron at a finite temperature

Bao-Quan Sun, Wei Xiao and Jing-Lin Xiao

Department of Physics, Inner Mongolia National Teacher's College, Tongliao 028043,
People's Republic of China

Received 21 December 1993, in final form 7 April 1994

Abstract. There is weak bulk but strong surface coupling between electrons and phonons for many polar crystals. In this paper, the influences of the electron interaction with both the weak-coupling bulk longitudinal optical and the strong-coupling surface optical phonons on the temperature characteristic of the surface polaron is discussed. The temperature dependences of the vibration frequency, the induced potential and the effective mass of the surface polaron were investigated using a linear-combination operator method. Numerical calculation, for a AgCl crystal, as an example, illustrates that the vibration frequency, the induced potential and the effective mass of the surface polaron will decrease with increasing temperature.

1. Introduction

In the early 1970s, Ibach [1] carried out low-energy electron diffraction (LEED) experiments on ZnO and other semiconductor surfaces. The surface or interface polarons in the crystals are of considerable interest. The behaviour of the electron–phonon interaction near the surface or interface of the dielectric layer has been studied by many workers [2, 3]. Recently, there have been some new investigations of the temperature dependence of the polaron mass [4–7]. In these theoretical studies, the different mechanisms of the electron–phonon interaction and the different theoretical approximation methods have provided two completely contrary conclusions. In early investigations, Yokota [8] found that the polaron mass decreases with increasing temperature using the Hartree approximation. However, using the Gurari variation method, Fulton [9] reached the opposite conclusion. Until now, the conclusions have not been identical. At low lattice temperatures, some theories [4, 5] predicted the same result as did Yokota, while others [6, 7] led to a polaron mass that increases with increasing temperature. The polaron mass in crystals is usually determined by cyclotron resonance experiments in a weak magnetic field. For different materials the experimental results also showed the same two contrary conclusions. The experimental data for the silver halides illustrated that the mass would increase as the lattice temperature increased [10]. In the cyclotron resonance measurements on GaAs–Ga_{1-x}Al_xAs heterojunctions Brummell *et al* [11] reported an anomalous case, i.e. the mass increases with increasing temperature up to about 100 K and starts to decrease for higher temperature.

Huybrechts [12] proposed a linear-combination operator method, by which a strong-coupling polaron was investigated. Later, many workers [13, 14] studied the strong-coupling polaron in many aspects by this method. On the basis of Huybrechts' work, Tokuda [15] added another variational parameter to the momentum operator and also evaluated the ground-state energy and effective mass of the bulk polaron. For the bulk polaron, the weak- and intermediate-coupling theories are applicable for the electron–bulk longitudinal optical

(LO) phonon coupling constant $\alpha_i < 6$ [16], whereas for the surface polaron this confinement is about 2.5 [17]. Hence, when the electron–surface optical (SO) phonon coupling constant satisfied $\alpha_s > 2.5$, the strong-coupling theory must be applied. There is weak coupling between the electron and the bulk LO phonon but strong coupling between the electron and the SO phonon for many polar crystals. So far, research into this has been very scarce. The properties of the surface or interface polaron in polar crystals have been discussed by the method of a linear-combination operator and a simple unitary transformation by one of the present authors and a co-worker [18].

In the past, most work on surface or interface polarons in polar crystals was devoted to the calculation of the ground-state energy and the effective mass of polarons at zero temperature, and to the discussion of the dependence of the polaron's properties on the electron–phonon coupling strength. In fact, the case of a finite temperature is more significant. In recent years there has been a renewed interest in the temperature dependence of the properties of surface or interface polarons.

The purpose of this present paper is to explore the effect of the electron–phonon interaction on the temperature behaviour of surface polarons. With both the weak coupling between the electron and bulk LO phonon and the strong coupling between the electron and SO phonon included, we obtain an expression for the effective mass of the surface polaron as a function of the temperature T and coordinate z and the temperature dependence of the induced potential of the surface polaron by using the linear-combination operator method. Numerical calculations, taking a AgCl crystal as an example, are performed and the temperature dependence of these quantities for the surface polaron in polar crystals are discussed.

2. The Hamiltonian

A surface between a AgCl crystal and vacuum is perpendicular to the z axis; the semi-infinite space $z > 0$ is occupied by the AgCl crystal, whereas the space $z < 0$ is a vacuum. A slow electron is placed inside the AgCl crystal at a distance $z (> 0)$ from the surface. We assume the effective-mass approximation to be valid and, for the slowly moving electron, the effect of small and finite penetration of the electron through the surface to be negligible. Because our interest is to investigate directly the temperature dependence of the polaron qualitatively, for simplicity we consider only the interaction between the electron and long-wavelength optical phonons without the influence of the electronic polarizability. With the above considerations, the Hamiltonian of the electron–phonon system in explicit form can be written as [17–19]

$$\begin{aligned}
 H = & \frac{p_{\parallel}^2}{2m} + \frac{p_z^2}{2m} + \frac{e^2(\epsilon_{\infty} - 1)}{4z\epsilon_{\infty}(\epsilon_{\infty} + 1)} + \sum_w \hbar\omega_L a_w^{\dagger} a_w + \sum_Q \hbar\omega_s b_Q^{\dagger} b_Q \\
 & + \sum_w \sin(w_z z) [V_w^* \exp(-i w_{\parallel} \cdot \rho) a_w^{\dagger} + \text{HC}] \\
 & + \sum_Q \exp(-Qz) (V_Q^* \exp(-i Q \cdot \rho) b_Q^{\dagger} + \text{HC}) \quad (1a)
 \end{aligned}$$

$$V_w^* = i \left(\frac{4\pi e^2 \hbar \omega_L}{\epsilon V} \right)^{1/2} \frac{1}{w} \quad (1b)$$

$$V_Q^* = i \left(\frac{\pi e^2 \hbar \omega_s}{\varepsilon^* S Q} \right)^{1/2} \quad (1c)$$

$$\frac{1}{\varepsilon} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \quad (1d)$$

$$\frac{1}{\varepsilon^*} = \frac{\varepsilon_0 - 1}{\varepsilon_0 + 1} - \frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 1} \quad (1e)$$

In (1a), the first two terms are the kinetic energies of the electron in the directions perpendicular and parallel to the surface of the crystals. The third term represents the energy of the image potential. The fourth and fifth terms in (1a) are the energies of the bulk LO and SO phonon fields, respectively. The last two terms describe the electron-bulk LO phonon and electron-SO phonon interaction energies. S and V are the surface area and the volume, respectively, of the AgCl crystal. m is the band mass of the electron and K is its wavevector (in (1a) the subscript \parallel denotes the projection of a given vector onto a plane parallel to the surface). ω_L and ω_s are frequencies of the bulk LO and SO phonons, respectively. In these expressions, a_w^+ and a_w are the creation and annihilation operators, respectively, of a bulk LO phonon with a three-dimensional wavevector w and b_Q^+ and b_Q are the corresponding operators for the SO phonon with a two-dimensional wavevector $Q \cdot p_{\parallel}$ and ρ are the momentum and the position vector, respectively, of an electron in a plane parallel to the surface. p_z and z are the momentum and position, respectively, of the electron in the z direction. ε_0 and ε_∞ are the static and high-frequency dielectric constants, respectively, of the crystal.

The Hamiltonian can formally be divided into two parts:

$$H = H_{\perp} + H_{\parallel} \quad (2a)$$

where

$$H_{\perp} = \frac{p_z^2}{2m} + \frac{e^2(\varepsilon_\infty - 1)}{4z\varepsilon_\infty(\varepsilon_\infty + 1)} \quad (2b)$$

and the rest is called H_{\parallel} . On the assumption that the motion in the z direction is slow, thus in determining the motion state in the x - y plane, quantities such as the momentum and position in the z direction may be regarded as parameters. This procedure is exactly analogous to the quasi-adiabatic approximation [20-22]. For motion parallel to the x - y plane we introduce the unitary transformations

$$U_1 = \exp \left[-i \left(\sum_w A_1 a_w^+ a_w w + \sum_Q A_2 b_Q^+ b_Q Q \right) \cdot \rho \right] \quad (3a)$$

$$U_2 = \exp \left(\sum_w (a_w^+ f_w - a_w f_w^*) + \sum_Q (b_Q^+ g_Q - b_Q g_Q^*) \right) \quad (3b)$$

where A_i ($i = 1, 2$) is a parameter characterizing the coupling strength. In the unitary transformation U_1 , $A_i = 1$ corresponds to the weak-coupling limit and $A_i = 0$ corresponds to the strong-coupling limit. f_w , f_w^* , g_Q and g_Q^* are variational parameters.

Following Tokuda [15] we also introduce the linear combination of the creation operator b_j^\dagger and annihilation operator b_j to represent the momentum and position of the electron:

$$p_{\parallel j} = \left(\frac{m\hbar\lambda}{2} \right)^{1/2} (b_j^\dagger + b_j + p_{0j}) \quad (4a)$$

$$p_j = i \left(\frac{\hbar}{2m\lambda} \right)^{1/2} (b_j - b_j^\dagger) \quad (4b)$$

where the subscript j refers to the x and y directions, λ and p_0 are the variational parameters, and b_j^\dagger and b_j are boson operators satisfying the boson commutative relation. Applying the transformations (3a) and (3b) to the Hamiltonian H_1 and using the operator expressions (4a) and (4b) and the fact that, in the unitary transformation U_1 , $A_1 = 1$ corresponds to the weak coupling between the electron and the bulk LO phonon and $A_2 = 0$ corresponds to the strong coupling between the electron and the surface LO, we can easily obtain

$$\begin{aligned} \mathcal{H}_{\parallel} = & U_2^{-1} U_1^{-1} H_1 U_1 U_2 = \frac{\hbar\lambda}{2} \left(\sum_j b_j^\dagger b_j + 1 \right) + \frac{\hbar\lambda}{4} \sum_j (b_j^\dagger b_j^\dagger + b_j b_j + p_{0j}^2) \\ & + \frac{\hbar\lambda}{2} \sum_j (b_j + b_j^\dagger) p_{0j} + \sum_w \left(\hbar\omega_L + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) (a_w^\dagger a_w + a_w^\dagger f_w + a_w f_w^* + |f_w|^2) \\ & + \sum_Q \hbar\omega_s (b_Q^\dagger b_Q + b_Q^\dagger g_Q + b_Q g_Q^* + |g_Q|^2) \\ & + \frac{\hbar^2}{2m} \sum_{w \neq w'} (a_w^\dagger + f_w^*) (a_{w'}^\dagger + f_{w'}^*) (a_w + f_w) (a_{w'} + f_{w'}) w_{\parallel} \cdot w'_{\parallel} \\ & - \hbar \left(\frac{\hbar\lambda}{2m} \right)^{1/2} \sum_w (a_w^\dagger a_w + a_w^\dagger f_w + a_w f_w^* + |f_w|^2) \sum_j (b_j^\dagger + b_j + p_{0j}) w_{\parallel j} \\ & + \sum_w \sin(w_z z) [V_w^* (a_w^\dagger + f_w^*) + \text{HC}] \\ & + \sum_Q \exp(-Qz) \left\{ V_Q^* (b_Q^\dagger + g_Q^*) \exp\left(-\frac{\hbar Q^2}{4m\lambda}\right) \right. \\ & \left. \times \exp\left[-\left(\frac{\hbar}{2m\lambda}\right)^{1/2} \sum_j b_j^\dagger Q_j\right] \exp\left[\left(\frac{\hbar}{2m\lambda}\right)^{1/2} \sum_j b_j Q_j\right] + \text{HC} \right\}. \quad (5) \end{aligned}$$

we choose a trial wavefunction for $|\phi\rangle$ at a finite temperature:

$$|\phi\rangle = |\phi(z)\rangle | \{n_j\} \rangle | \{n_w\} \{n_Q\} \rangle \quad (6)$$

where $|\phi(z)\rangle$ is the wavefunction in the z direction. $|\{n_j\}\rangle$ and $|\{n_w\}\{n_Q\}\rangle$ are the wavefunctions for describing the polaron and phonon states, in which $\{n_j\}$, $\{n_w\}$ and $\{n_Q\}$ represent the numbers of surface polarons, bulk LO phonons and SO phonons, respectively. In the occupation number picture we have

$$\begin{aligned} b_j^\dagger |n_j\rangle &= \sqrt{n_j + 1} |n_j + 1\rangle & b_j |n_j\rangle &= \sqrt{n_j} |n_j - 1\rangle \\ a_w^\dagger |n_w\rangle &= \sqrt{n_w + 1} |n_w + 1\rangle & a_w |n_w\rangle &= \sqrt{n_w} |n_w - 1\rangle \\ b_Q^\dagger |n_Q\rangle &= \sqrt{n_Q + 1} |n_Q + 1\rangle & b_Q |n_Q\rangle &= \sqrt{n_Q} |n_Q - 1\rangle. \end{aligned} \quad (7)$$

3. The effective Hamiltonian and the effective mass

In the variation for minimizing the ground-state energy with respect to the variational parameter and the functions mentioned above, the system must be constrained by the conservation of total momentum. However, in the adiabatic approximation, the momentum in the z direction is regarded as a parameter; so it is only constrained by the total momentum parallel to the x - y plane;

$$\mathbf{p}_{\parallel T} = \mathbf{p}_{\parallel} + \sum_w \hbar \omega_w a_w^{\dagger} a_w + \sum_Q \hbar Q b_Q^{\dagger} b_Q. \quad (8)$$

The minimization problem is now carried out by the use of the Lagrange multipliers. Choosing an arbitrary constant multiplier u , we have

$$\langle \phi | (\mathcal{H}_{\parallel} - U_2^{-1} U_1^{-1} \mathbf{u} \cdot \mathbf{p}_{\parallel T} U_1 U_2) | \phi \rangle = \langle \phi(z) | F(\lambda, f_w, g_Q, u, p_0) | \phi(z) \rangle \quad (9a)$$

where

$$\begin{aligned} F(\lambda, f_w, g_Q, u, p_0) &= \langle \{n_Q\} | \langle \{n_w\} | \langle \{n_j\} | (\mathcal{H}_{\parallel} - U_2^{-1} U_1^{-1} \mathbf{u} \cdot \mathbf{p}_{\parallel T} U_1 U_2) | \{n_j\} \rangle | \{n_w\} \rangle | \{n_Q\} \rangle \\ &= (n + \frac{1}{2}) \hbar \lambda + \frac{\hbar \lambda}{4} p_0^2 + \sum_Q \hbar \omega_s (n_Q + |g_Q|^2) + \sum_w \hbar \omega_l (n_w + |f_w|^2) \\ &\quad - \left(\frac{m \hbar \lambda}{2} \right)^{1/2} \mathbf{p}_0 \cdot \mathbf{u} + \frac{\hbar^2}{2m} \sum_w \omega^2 (n_w + |f_w|^2) \\ &\quad - \sum_Q \hbar \mathbf{Q} \cdot \mathbf{u} (n_Q + |g_Q|^2) - \hbar \left(\frac{\hbar \lambda}{2m} \right)^{1/2} \sum_w (n_w + |f_w|^2) \omega_w \cdot \mathbf{p}_0 \\ &\quad + \sum_w \sin(\omega_w z) (V_w^* f_w^* + \text{HC}) \\ &\quad + \sum_Q \exp(-Qz) \left[V_Q^* g_Q^* \exp\left(-\frac{\hbar Q^2}{4m\lambda}\right) B(n) + \text{HC} \right] \end{aligned} \quad (9b)$$

$$\begin{aligned} B(n) &= \langle \{n_j\} | \exp \left[- \left(\frac{\hbar}{2m\lambda} \right)^{1/2} \sum_j b_j^{\dagger} Q_j \right] \exp \left[\left(\frac{\hbar}{2m\lambda} \right)^{1/2} \sum_j b_j Q_j \right] | \{n_j\} \rangle \\ &= 1 - n \frac{\hbar Q^2}{2m\lambda} + O \left(\frac{\hbar Q^2}{2m\lambda} \right)^2. \end{aligned} \quad (9c)$$

$F(\lambda, f_w, g_Q, u, p_0)$ may be called the variational parameter function. Minimizing (9b) with respect to λ, f_w, g_Q, u and p_0 , we can determine these parameters and functions. In the calculation procedures above, we have considered the symmetry of the electron moving in the x - y plane, with $n_x = n_y = n$, and neglected the higher-order small quantity terms of the wavevector. For weak coupling between the electron and bulk LO phonons, we also neglected the interaction of the phonons with different wavevectors due to recoil. Using the variational method, we get

$$f_w = - \frac{V_w^* \sin(\omega_w z)}{\hbar^2 \omega_w^2 / 2m + \hbar \omega_l - \hbar (\hbar \lambda / 2m)^{1/2} \mathbf{p}_0 \cdot \omega_{\parallel}} \quad (10a)$$

$$g_Q = - \frac{\exp(-Qz) V_Q^* \exp(-\hbar Q^2 / 4m\lambda) B(n)}{\hbar \omega_s - \hbar \mathbf{Q} \cdot \mathbf{u}} \quad (10b)$$

and their complex conjugate expressions. Substituting (10) into (9b), we have

$$\begin{aligned}
 F(\lambda, u, p_0) = & (n + \frac{1}{2})\hbar\lambda + \frac{\hbar\lambda}{4}p_0^2 + \sum_w \left(\hbar\omega_l + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) n_w \\
 & + \sum_Q (\hbar\omega_s - \hbar\mathbf{Q} \cdot \mathbf{u}) n_Q - \left(\frac{m\hbar\lambda}{2} \right)^{1/2} p_0 \cdot \mathbf{u} - \hbar \left(\frac{\hbar\lambda}{2m} \right)^{1/2} \sum_w n_w p_0 \cdot \mathbf{w}_{\parallel} \\
 & - \sum_w \frac{|V_w|^2 \sin^2(w_z z)}{\hbar^2 w_{\parallel}^2 / 2m + \hbar\omega_l - \hbar(\hbar\lambda/2m)^{1/2} p_0 \cdot \mathbf{w}_{\parallel}} \\
 & - \sum_Q \frac{|V_Q|^2 \exp(-2Qz) B^2(n)}{\hbar\omega_s - \hbar\mathbf{Q} \cdot \mathbf{u}} \exp\left(-\frac{\hbar Q^2}{2m\lambda}\right). \tag{11}
 \end{aligned}$$

The final two terms in (11) can be calculated by replacing the summation with integration and expanding them up to the second-order term of u and p_0 for a slow electron. In this expression, the first-order terms in $p_0 \cdot \mathbf{w}_{\parallel}$ and $\mathbf{Q} \cdot \mathbf{u}$ are equal to zero; thus, we have

$$\begin{aligned}
 F(\lambda, u, p_0) = & (n + \frac{1}{2})\hbar\lambda + \frac{\hbar\lambda}{4}p_0^2 + \sum_Q n_Q \hbar\omega_s + \sum_w \left(\hbar\omega_l + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) n_w \\
 & - \left(\frac{m\hbar\lambda}{2} \right)^{1/2} p_0 \cdot \mathbf{u} - \alpha_l \hbar\omega_l \left(\frac{\pi}{2} - K(z) \right) - \frac{\alpha_l \hbar\lambda}{2} p_0^2 \left(\frac{\pi}{16} - L(z) \right) \\
 & - \alpha_s \hbar(\omega_s \lambda)^{1/2} M(z) - \alpha_s \left(\frac{\lambda}{\omega_s} \right)^{3/2} m u^2 N(z) \tag{12a}
 \end{aligned}$$

$$K(z) = \int_0^{\infty} \frac{\exp(-2zu_l x)}{1+x^2} dx \tag{12b}$$

$$L(z) = \int_0^{\infty} \frac{x^2 \exp(-2zu_l x)}{(1+x^2)^3} dx \tag{12c}$$

$$M(z) = \int_0^{\infty} (1-2nx^2) \exp(-x^2 - 2zu_{\lambda} x) dx \tag{12d}$$

$$N(z) = \int_0^{\infty} x^2 \exp(-x^2 - 2zu_{\lambda} x) dx \tag{12e}$$

$$\begin{aligned}
 \alpha_l = \frac{me^2}{\varepsilon \hbar^2 u_l} \quad \alpha_s = \frac{me^2}{\varepsilon^* \hbar^2 u_s} \quad u_l = \left(\frac{2m\omega_l}{\hbar} \right)^{1/2} \\
 u_s = \left(\frac{2m\omega_s}{\hbar} \right)^{1/2} \quad u_{\lambda} = \left(\frac{2m\lambda}{\hbar} \right)^{1/2}. \tag{12f}
 \end{aligned}$$

The extremum condition $\partial F / \partial p_0 = 0$ gives

$$\rho_0 = \frac{(2m/\hbar\lambda)^{1/2}}{1 - (\pi/8)\alpha_l + 2\alpha_l L(z)} u. \tag{13}$$

Substituting (13) into (12a), we get

$$\begin{aligned}
 F(\lambda, u) = & (n + \frac{1}{2})\hbar\lambda + \sum_Q n_Q \hbar\omega_s + \sum_w n_w \left(\hbar\omega_l + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) \\
 & - \alpha_l \hbar\omega_l \left(\frac{\pi}{2} - K(z) \right) - \alpha_s \hbar(\omega_s \lambda)^{1/2} M(z) \\
 & - \frac{1}{2} m u^2 \left[\frac{1}{1 - (\pi/8)\alpha_l + 2\alpha_l L(z)} + 2\alpha_s \left(\frac{\lambda}{\omega_s} \right)^{3/2} N(z) \right]. \tag{14}
 \end{aligned}$$

For a slow electron, u is very small; one can omit the final term in (14) so that the variation in $F(\lambda, u)$ with respect to λ yields

$$\sqrt{\lambda} = \alpha_s \sqrt{\omega_s} \int_0^\infty \frac{1 - 2nx^2}{2n + 1} (1 - 2zu_\lambda x) \exp(-x^2 - 2zu_\lambda x) dx. \tag{15}$$

For the momentum expectation value of the surface polaron we find

$$\begin{aligned}
 p_{\parallel} = & \langle \{n_Q\} | \langle \{n_w\} | \langle \{n_j\} | U_2^{-1} U_1^{-1} p_{\parallel} U_1 U_2 | \{n_j\} \rangle | \{n_w\} \rangle | \{n_Q\} \rangle \\
 = & m \left[\frac{1}{1 - (\pi/8)\alpha_l + 2\alpha_l L(z)} + 2\alpha_s \left(\frac{\lambda}{\omega_s} \right)^{3/2} N(z) \right] u. \tag{16a}
 \end{aligned}$$

It is evident from the structure of this expression that u has the meaning of velocity which may be regarded as the average velocity of the surface polaron in the x - y plane, and the factor before u , namely

$$m^* = m \left[\frac{1}{1 - (\pi/8)\alpha_l + 2\alpha_l L(z)} + 2\alpha_s \left(\frac{\lambda}{\omega_s} \right)^{3/2} N(z) \right] \tag{16b}$$

can be interpreted as the effective mass of the surface polaron.

The effective Hamiltonian of the surface polaron can be represented as

$$\begin{aligned}
 H_{\text{eff}} = & H_{\perp} + \min(\langle n_Q \rangle | \langle \{n_w\} | \langle \{n_j\} | \mathcal{H}_{\parallel} | \{n_j\} \rangle | \{n_w\} \rangle | \langle n_Q \rangle) \\
 = & \frac{p_z^2}{2m} + \frac{p_{\parallel}^2}{2m^*} + \frac{e^2(\epsilon_{\infty} - 1)}{4z\epsilon_{\infty}(\epsilon_{\infty} + 1)} + (n + \frac{1}{2})\hbar\lambda + \sum_Q n_Q \hbar\omega_s \\
 & + \sum_w n_w \left(\hbar\omega_l + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) - \alpha_l \hbar\omega_l \left(\frac{\pi}{2} - K(z) \right) - \alpha_s \hbar(\omega_s \lambda)^{1/2} M(z). \tag{17}
 \end{aligned}$$

we now consider two limiting cases.

(1) The electron is very near the surface, i.e. $z \ll u_i^{-1}$ or u_s^{-1} . In this case, we have

$$\lambda = \frac{\pi}{4} \left(\frac{1 - n}{2n + 1} \right)^2 \alpha_s^2 \omega_s^2 \tag{18a}$$

$$m^* = m \left[1 - \frac{\pi^2}{16} \left(\frac{1 - n}{2n + 1} \right)^3 \alpha_s^4 \right] \tag{18b}$$

$$\begin{aligned}
 H_{\text{eff}} = & \frac{p_z^2}{2m} + \frac{p_{\parallel}^2}{2m^*} + \frac{e^2(\epsilon_{\infty} - 1)}{4z\epsilon_{\infty}(\epsilon_{\infty} + 1)} + \sum_Q n_Q \hbar\omega_s \\
 & + \sum_w n_w \left(\hbar\omega_l + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) - \frac{\pi}{8} \frac{(1 - n)^2}{2n + 1} \alpha_s^2 \hbar\omega_s. \tag{18c}
 \end{aligned}$$

From (18) one can see that the effective mass and the effective Hamiltonian of the surface polaron are independent of the interaction between the electron and the bulk LO phonon whereas they are dependent on the interaction between the electron and the SO phonon. The increasing part of the effective mass of the surface polaron is proportional to α_s^4 because of the interaction between the electron and the SO phonon. The self-trapping energy is $(\pi/8)[(1-n)^2/2n+1]\alpha_s^2\hbar\omega_s$, and proportional to α_s^2 . The self-trapping energy will decrease when the temperature increases. It is induced by the polarization of SO vibration only. In the low-temperature limit $n_w = n_Q = n = 0$, our results are identical with that of Hipolito [23] and that in [18].

(2) The electron is very deep in the bulk, i.e. $z \gg u_l^{-1}$ or u_s^{-1} . In this case, we have

$$\lambda = 0 \quad (19a)$$

$$m^* = \frac{m}{1 - (\pi/8)\alpha_l} \quad (19b)$$

$$H_{\text{eff}} = \frac{p_z^2}{2m} + \frac{p_{\parallel}^2}{2m^*} + \frac{e^2(\epsilon_0 - 1)}{4z\epsilon_0(\epsilon_0 + 1)} + \sum_Q n_Q \hbar\omega_s + \sum_w n_w \left(\hbar\omega_l + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) - \frac{\pi}{2} \alpha_l \hbar\omega_l. \quad (19c)$$

The effective mass and the effective Hamiltonian of the surface polaron are only dependent on the interaction between the electron and bulk LO phonon. The self-trapping energy is $(\pi/2)\alpha_l \hbar\omega_l$ and proportional to α_l . In the low-temperature limit $n_w = n_Q = n = 0$, our results are identical with those of [18, 20].

4. Temperature dependence of the surface polaron

At a finite temperature, the electron system is no longer in the ground state entirely. The lattice vibrations excite not only real phonons but also electrons in a parabolic potential well. The properties of the polaron are a statistical average of the electron-phonon system in various states. As shown in [18], the phonon frequencies will decrease with increasing temperature but, if the temperature is restricted to a range lower than room temperature ($T < 300$ K), the relative change ($|\Delta\omega|/\omega$) in the frequency is only 1%. Then we can take the phonon frequencies as approximately constant. With the consideration mentioned above, we assume that the eigenvalues of $a_w^+ a_w$ and $b_Q^+ b_Q$ in the phonon state at a finite temperature are given by the Planck distribution functions. According to quantum statistics, we have

$$\bar{n} = \left[\exp\left(\frac{\hbar\lambda}{k_B T}\right) - 1 \right]^{-1} \quad (20a)$$

$$\bar{n}_w = \left[\exp\left(\frac{\hbar\omega_l}{k_B T}\right) - 1 \right]^{-1} \quad (20b)$$

$$\bar{n}_Q = \left[\exp\left(\frac{\hbar\omega_s}{k_B T}\right) - 1 \right]^{-1} \quad (20c)$$

where k_B is the Boltzmann constant.

However, the value of λ determined by (15) relates not only to the value of z but also to the value of \bar{n} , which should be self-consistent with (20). Substituting (20) into (15), we can obtain the relation of λ to z and T . Finally, the effective Hamiltonian of the surface polaron can be expressed as

$$H_{\text{eff}} = \frac{p_z^2}{2m} + \frac{P_{\parallel}^2}{2m^*} + (\bar{n} + \frac{1}{2})\hbar\lambda + \sum_Q n_Q \hbar\omega_s + \sum_w n_w \left(\hbar\omega_l + \frac{\hbar^2 w_{\parallel}^2}{2m} \right) + V_{\text{img}} + V_i^{\text{b}} + V_i^{\text{s}} \tag{21a}$$

where

$$V_{\text{img}} = \frac{e^2(\epsilon_{\infty} - 1)}{4z\epsilon_{\infty}(\epsilon_{\infty} + 1)} \tag{21b}$$

$$V_i^{\text{b}} = -\alpha_l \hbar\omega_l \left(\frac{\pi}{2} - K(z) \right) \tag{21c}$$

$$V_i^{\text{s}} = -\alpha_s \hbar(\omega_s \lambda)^{1/2} M(z) \tag{21d}$$

are the image potential, the potential induced by the electron-LO phonon interaction and the potential induced by the electron-SO interaction, respectively. The effective potential is defined as

$$V_{\text{eff}} = V_{\text{img}} + V_i^{\text{b}} + V_i^{\text{s}}. \tag{21e}$$

Following Liang [20] we define the ‘dead layer’ of the surface polaron. Its thickness is determined by

$$V_{\text{eff}}|_{z=d} = 0. \tag{22}$$

Evidently, both the induced potential and the thickness of the dead layer of surface polarons depend on the temperature.

Table 1. The data for a AgCl crystal. All the parameters are taken from [24].

Material	ϵ_0	ϵ_{∞}	$\hbar\omega_l$ (meV)	$\hbar\omega_s$ (meV)	α_l	α_s
AgCl	9.5	3.97	23.0	21.6	1.97	2.89

5. Results and discussion

In this section, taking the polaron in the surface of a AgCl crystal as an example, we perform a numerical evaluation. In table 1, the data for a AgCl crystal are given. Figure 1 shows the variation in the frequency λ of the surface polaron in a AgCl crystal with the coordinate z at different temperatures. The solid curve denotes the case $T = 100$ K, and the broken curve represents the case of zero temperature. From the figure, one can see that the frequency λ will decrease with increasing z . At the same position (same value of z),

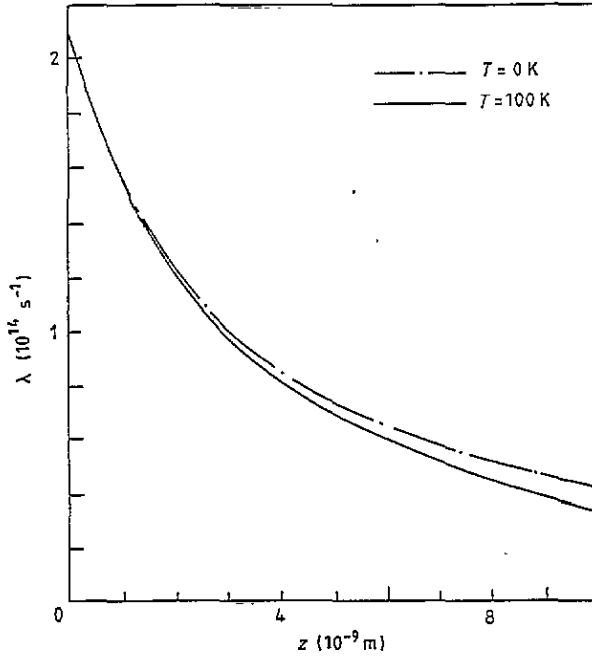


Figure 1. The relation between λ and z in a AgCl crystal at different temperatures.

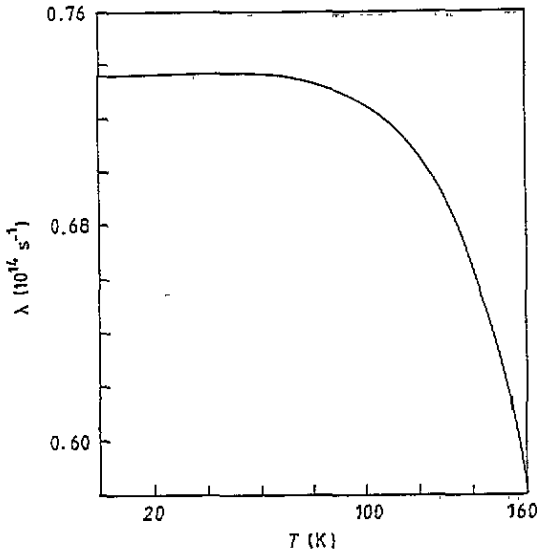


Figure 2. The relation between λ and T at a certain coordinate $z = 5 \times 10^{-9}$ m.

the higher the temperature, the smaller is the value of λ . From figure 1, one can also see that the frequency of the surface polaron will decrease with increasing temperature. The dependence of the vibrational frequency of the polaron for a AgCl crystal on temperature at a certain coordinate $z = 5 \times 10^{-9}$ m is plotted in figure 2. From figure 2, we also

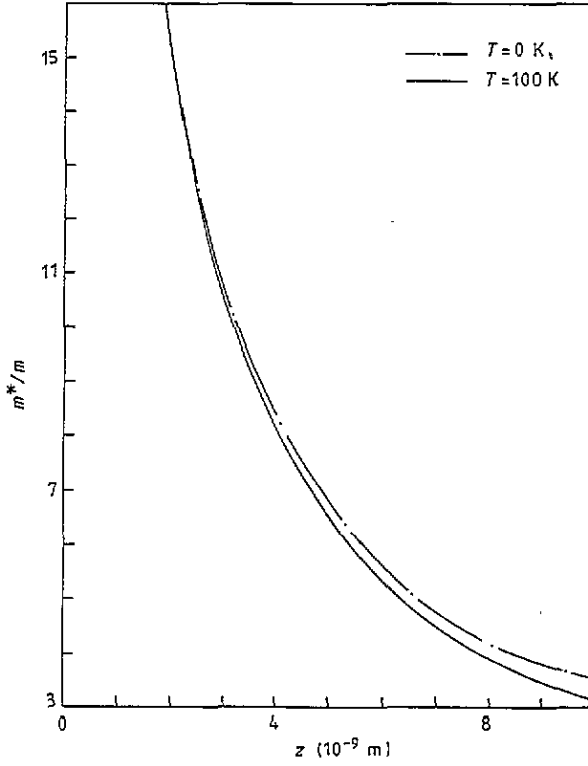


Figure 3. The relation between m^*/m and z at different temperatures.

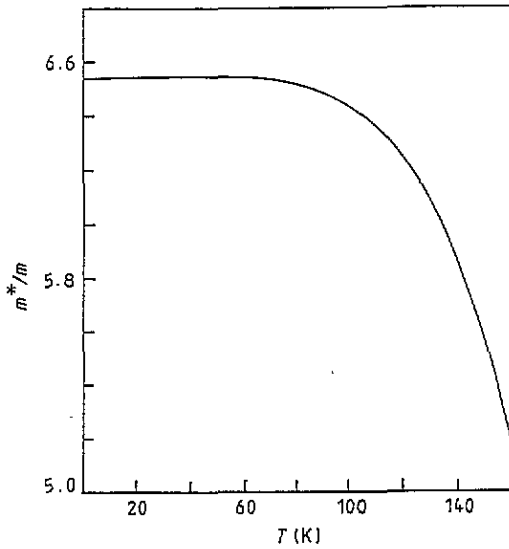


Figure 4. The relation between m^*/m and T at a certain coordinate $z = 5 \times 10^{-9}$ m.

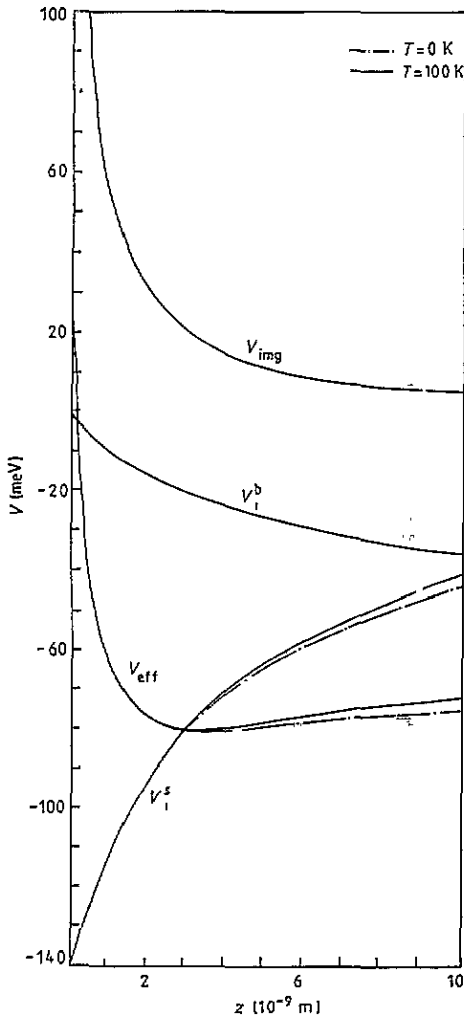


Figure 5. The relation between the image potential V_{img} and induced potentials V_I^s and V_I^b and z in a AgCl crystal at different temperatures T .

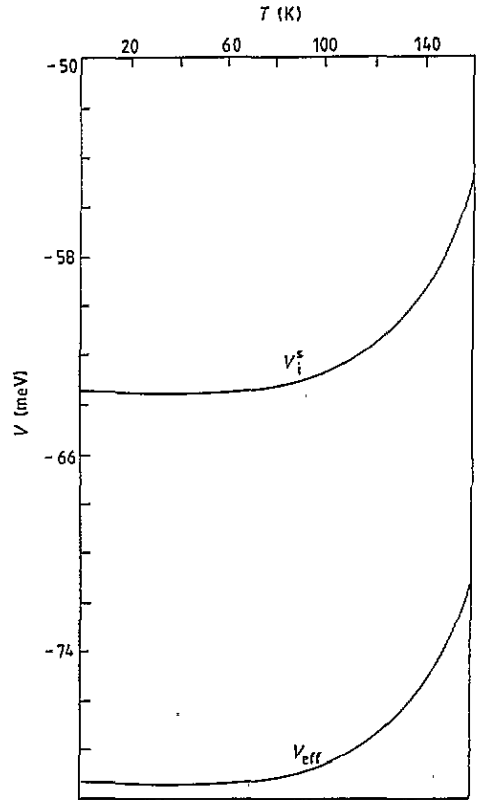


Figure 6. The relation between the induced potential V_I^s and effective potential V_{eff} and T at a certain coordinate $z = 5 \times 10^{-9}$ m.

see that the vibrational frequency of the surface polaron changes little with temperature for $T < 80$ K, whereas it changes strongly with temperature for $T > 80$ K.

Figure 3 shows the relation between the effective mass m^*/m and the coordinate z at different temperatures T . The broken curve denotes the case of zero temperature, and the solid curve represents the case $T = 100$ K. From the figure, one can see that, as a result of the temperature behaviour of the electron-phonon interaction, the value of the effective mass m^*/m will decrease with increasing temperature at the same value of the coordinate z . Figure 4 give the relationship between the effective mass m^*/m in a AgCl crystal and the temperature T at a certain coordinate $z = 5 \times 10^{-9}$ m. Figure 4 also shows that the effective mass of the surface polaron changes little with temperature for $T < 80$ K, whereas it changes strongly with temperature for $T > 80$ K. From (18b) we find that in the two-dimensional limit ($z \rightarrow 0$) the temperature behaviour of the polaron mass is really attributed

to the SO mode effect.

Figure 5 show the relationship between the image potential V_{img} , the induced potential V_i^b resulting from the electron–bulk LO phonon interaction, the induced potential V_i^s resulting from the electron–SO phonon interaction and the effective potential V_{eff} in a AgCl crystal with the coordinate z at different temperatures T . The solid curve denotes the case $T = 100$ K, and the broken curve represents the case of zero temperature. It is indicated that there is only a temperature dependence of the electron–SO phonon interaction, whereas the image potential and the electron–bulk LO phonon interaction are independent of temperature. It can be seen from figure 5 that V_i^b increases with increase in z , whereas V_i^s increases with decreasing z . Near the surface, the electron–SO phonon interaction is dominant, whereas in the bulk far from surface of the electron–bulk LO phonon interaction is dominant. The curve of the effective potential of the surface polaron is also drawn in figure 5. As $z \rightarrow 0$, the surface polaron is repelled away from the surface, i.e. the surface polaron is not able to exist near the surface. Thus the surface polaron cannot get infinitely near to the surface; there is no polaron in the range near the surface ($V_{\text{eff}} > 0$). Because of the similarity to the case of excitons we call the thin layer the surface polaron-free surface layer (SPFSL) or the dead layer of surface polarons. Solving the equation

$$V_{\text{eff}}(z) = 0 \quad (23)$$

the root is the depth of the SPFSL, which we denote as d (for a AgCl crystal, $d = 1.27 \text{ \AA}$). From figure 5, we also see that the induced potential V_i^s and the effective potential V_{eff} in a AgCl crystal will decrease with rise in temperature. Figure 6 show the relationship between the induced potential V_i^s and the effective potential V_{eff} with temperature T at a certain coordinate ($z = 5 \times 10^{-9} \text{ m}$). From figure 6, we also see that the induced potential V_i^s and the effective potential V_{eff} of the surface polaron change little with temperature for $T < 80$ K, whereas they change strongly with temperature for $T > 80$ K.

Acknowledgment

This project was supported by the Laboratory of Excited State Processes, Changchun Institute of Physics.

References

- [1] Ibach H 1970 *Phys. Rev. Lett.* **24** 141; 1971 *Phys. Rev. Lett.* **27** 253
- [2] Lucas A A, Kartheuser E and Badro R G 1970 *Phys. Rev. B* **2** 2485
- [3] Evans E and Mills D L 1972 *Solid State Commun.* **11** 1093; 1973 *Phys. Rev. B* **8** 4004
- [4] Saitoh M 1980 *J. Phys. Soc. Japan* **49** 878, 886
- [5] Arisawa K and Saitoh M 1983 *Phys. Status Solidi b* **120** 361
- [6] Peeters F M and Devreese J T 1982 *Phys. Rev. B* **25** 7302; 1985 *Phys. Rev. B* **31** 5300
- [7] Fedyanin V K and Rodriguez C 1982 *Phys. Status Solidi b* **110** 105
- [8] Yokota T 1983 *Busseiron-kenkyu* **69** 137
- [9] Fulton T 1956 *Phys. Rev.* **103** 1712
- [10] Masumi T 1984 *Polarons and Excitons in Semiconductor and Ionic Crystals* ed J T Devreese and F M Peeters (New York: Plenum) p 99
- [11] Brummell M A, Nicholas R J, Hopkins M A, Harris J J and Foxon C T 1987 *Phys. Rev. Lett.* **58** 77
- [12] Huybrechts J 1976 *J. Phys. C: Solid State Phys.* **9** L211
- [13] Tokuda N 1980 *J. Phys. C: Solid State Phys.* **13** L173
- [14] Gu S W and Zheng J 1984 *Phys. Status Solidi b* **121** K165

- [15] Tokuda N 1980 *J. Phys. C: Solid State Phys.* **13** L851
- [16] Haga E 1954 *Prog. Theor. Phys.* **11** 449
- [17] Pan J S 1985 *Phys. Status Solidi b* **127** 307
- [18] Xiao J L and Gu S W 1988 *J. Neimenggu Univ.* **19** 52 (in Chinese)
Xiao J L 1991 *J. Hebei Normal Univ.* **35** 27 (in Chinese)
- [19] Li Y C and Gu S W 1990 *J. Phys.: Condens. Matter* **2** 1149
- [20] Liang X X and Gu S W 1984 *Solid State Commun.* **50** 505
- [21] Wei B H and Gu S W 1991 *Phys. Rev. B* **43** 9190
- [22] Wei B H, Liu Y Y and Gu S W 1991 *Phys. Rev. B* **44** 5703
- [23] Hipolito O 1979 *Solid State Commun.* **32** 515
- [24] Kartheuser E 1972 *Polarons in Ionic Crystals and Polar Semiconductors* (Amsterdam: North-Holland)