IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

The effective mass of a slow-moving surface polaron in a semi-infinite crystal

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

1997 J. Phys.: Condens. Matter 9 10567

(http://iopscience.iop.org/0953-8984/9/48/003)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.209
The article was downloaded on 14/05/2010 at 11:39

Please note that terms and conditions apply.

J. Phys.: Condens. Matter **9** (1997) 10567–10579. Printed in the UK PII: S0953-8984(97)84254-3

The effective mass of a slow-moving surface polaron in a semi-infinite crystal

Jing-Lin Xiao and Wei Xiao

Chinese Centre of Advanced Science and Technology (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China, Laboratory of Excited State Processes, Changchun Institute of Physics, Academia Sinica, Changchun 130021, People's Republic of China, and Department of Physics, Inner Mongolia National Teacher's College, Tongliao 028043, People's Republic of China†

Received 13 May 1997, in final form 18 August 1997

Abstract. There is weak bulk but strong surface coupling between electrons and phonons in a semi-infinite crystal. Here some properties of the surface polaron in a semi-infinite crystal, weak coupling with bulk longitudinal optical (BO) phonons and strong coupling with surface longitudinal optical (SO) phonons, are studied. The effective Hamiltonian of a slow-moving surface polaron in a semi-infinite crystal is derived using an improved linear combination operator and perturbation method. If we consider the interaction between phonons of different wave vectors in the recoil process, the influence of this interaction on the effective Hamiltonian, the induced potential and the effective mass of the surface polaron are discussed. Numerical calculations for an AgBr crystal, as an example, are performed, and some properties of the surface polaron in a semi-infinite crystal are discussed.

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 a crystal has been studied by many investigators [2–4]. Evans and Mills [5], using a variational approach, investigated the case where the electron interacted with both surface and bulk LO waves and the phonons were considered as the only electric-dipole active excitations. Gu *et al* [6, 7] discussed the ideal surface polaron and the weak, intermediate-coupling polaron in a semi-infinite polar crystal by means of the perturbation method.

Huybrechts [8] proposed a linear combination operator method, by which a strong-coupling polaron was investigated. Later, other authors [9–11] studied many aspects of the strong-coupling polaron by this method. On the basis of Huybrechts' work, Tokuda [12] added another variational parameter to the momentum operator and also evaluated the ground-state energy and effective mass of the bulk polaron. In fact, so far research on the polaron has been restricted to approximation and calculation where the interaction between phonons of different wave vectors in the recoil process is neglected. The properties of

† Address for correspondence.

0953-8984/97/4810567+13$19.50 © 1997 IOP Publishing Ltd

the surface polaron, considering the corresponding interaction, have been discussed by the perturbation method by the present authors and co-workers [13].

For the bulk polaron, the weak- and intermediate-coupling theories are applicable for the electron–bulk longitudinal optical phonon coupling constant $\alpha_l < 6$ [14], whereas for the surface polaron this confinement is about 2.5 [3]. Hence, when the electron–surface optical phonon coupling constant satisfies $\alpha_s > 2.5$, the strong-coupling theory must be applied. There is weak coupling between the electron and the bulk longitudinal optical phonon, but strong coupling between the electron and the surface optical phonon for many polar crystals. So far, research into this has been very scarce.

In this paper, the effect of the interaction between phonons of different wave vectors in the recoil process on the properties of the surface polaron in a semi-infinite crystal are studied by using an improved linear combination operator and perturbation method. 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 Hamiltonian of the surface polaron. If we consider the interaction between phonons of different wave vectors in the recoil process, the influence on the effective Hamiltonian, induced potential, effective interaction potential and effective mass of the surface polaron are investigated. Numerical calculations, taking the AgBr crystal example, are performed and the properties of these quantities for the surface polaron in a semi-infinite crystal are discussed.

2. Hamiltonian

A surface between an AgBr crystal and vacuum is perpendicular to the z axis; the semi-infinite space $z > 0$ is occupied by the AgBr crystal, whereas the space $z < 0$ is a vacuum. We consider a slow electron moving in an AgBr crystal which occupies the half space $z > 0$. Using the Hamiltonian of the interaction between an electron and SO phonons and bulk LO phonons that has been given by Evans and Mills [5], including the surface repulsive image potential with dielectric constant $\varepsilon_\infty(\neq 1)$ from the polarization of the electron cloud, the Hamiltonian of the electron–phonon system in explicit form can be written as ($\hbar = m = 1$; m is the band mass of the electron)

$$H = \frac{P_\parallel^2}{2} + \frac{P_z^2}{2} + \frac{e^2(\varepsilon_\infty - 1)}{4z\varepsilon_\infty(\varepsilon_\infty + 1)} + \sum_{\boldsymbol{W}} \omega_l a_{\boldsymbol{W}}^+ a_{\boldsymbol{W}} + \sum_{\boldsymbol{Q}} \omega_s b_{\boldsymbol{Q}}^+ b_{\boldsymbol{Q}} + \sum_{\boldsymbol{W}} \sin(w_z z)(V_{\boldsymbol{W}}^* \, \mathrm{e}^{-\mathrm{i}\boldsymbol{W}_\parallel \cdot \boldsymbol{\rho}} a_{\boldsymbol{W}}^+ + \mathrm{HC}) + \sum_{\boldsymbol{Q}} \mathrm{e}^{-QZ}(V_{\boldsymbol{Q}}^* \, \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{\rho}} \, b_{\boldsymbol{Q}}^+ + \mathrm{HC}) \tag{1a}$$

$$V_{\boldsymbol{W}}^* = \mathrm{i}\left(\frac{4\pi e^2 \omega_l}{\varepsilon V}\right)^{\frac{1}{2}} \frac{1}{W} \tag{1b}$$

$$V_{\boldsymbol{Q}}^* = \mathrm{i}\left(\frac{\pi e^2 \omega_s}{\varepsilon^* S}\right)^{\frac{1}{2}} \tag{1c}$$

$$\frac{1}{\varepsilon} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \tag{1d}$$

$$\frac{1}{\varepsilon^*} = \frac{\varepsilon_0 - 1}{\varepsilon_0 + 1} = \frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 1}. \tag{1e}$$

In (1*a*), $a_{\boldsymbol{W}}^{+}(a_{\boldsymbol{W}})$ is the creation (annihilation) operator of a bulk LO phonon with three-dimensional wave vector $\boldsymbol{W}$, $b_{\boldsymbol{Q}}^{+}(b_{\boldsymbol{Q}})$ is the corresponding operator for the SO phonon with two-dimensional wave vector $\boldsymbol{Q}$. $\boldsymbol{P}_{\parallel}$ and $\boldsymbol{\rho}$ are the momentum and 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. ω_l and ω_s are the frequencies of the bulk LO and SO phonons. S and V are the surface area and the volume of the crystal. ε_0 and ε_∞ are, respectively, the static and high-frequency dielectric constant of the crystal (in (1*a*) the subscript $\parallel$ denotes the projection of a given vector onto a plane parallel to the surface).

The Hamiltonian can formally be divided into two parts:

$$H = H_z + H_{\parallel} \tag{2a}$$

where

$$H_z = \frac{P_z^2}{2} + \frac{e^2(\varepsilon_\infty - 1)}{4z\varepsilon_\infty(\varepsilon_\infty + 1)} \tag{2b}$$

and the rest is called $H_{\parallel}$. Assuming the motion in the z direction to be slow, in determining the motion state in the x–y plane, the 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 [7, 15, 16]. We calculate $H_{\parallel}$, then add the calculated result to H_z so as to obtain the effective Hamiltonian of the system. For the motion parallel to the x–y plane we introduce unitary transformations to the Hamiltonian $H_{\parallel}$ with

$$U_1 = \exp\left(-\mathrm{i}\left(\sum_{\boldsymbol{W}} A_1 a_{\boldsymbol{W}}^{+} a_{\boldsymbol{W}} \boldsymbol{W}_{\parallel} + \sum_{\boldsymbol{Q}} A_2 b_{\boldsymbol{Q}}^{+} b_{\boldsymbol{Q}} \boldsymbol{Q} \right) \cdot \boldsymbol{\rho} \right) \tag{3a}$$

$$U_2 = \exp\left(\sum_{\boldsymbol{W}} (a_{\boldsymbol{W}}^{+} f_W - a_{\boldsymbol{W}} f_W^{*}) + \sum_{\boldsymbol{Q}} (b_{\boldsymbol{Q}}^{+} g_Q - b_{\boldsymbol{Q}} g_Q^{*}) \right) \tag{3b}$$

where $f_W(f_W^{*})$ and $g_Q(g_Q^{*})$ are variational parameters. $A_i (i = 1, 2)$ 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.

Following Tokuda [12] we also introduce the linear combination of the creation operator b_j^{+} and annihilation operator b_j to represent the momentum and position of the electron:

$$P_{\parallel j} = \left(\frac{\lambda}{2}\right)^{\frac{1}{2}} (b_j + b_j^{+} + P_{0j}) \tag{4a}$$

$$\rho_j = \mathrm{i}\left(\frac{1}{2\lambda}\right)^{\frac{1}{2}} (b_j - b_j^{+}) \tag{4b}$$

where the subscript j refers to the x and y directions, λ and P_0 are the variational parameters, and b_j^{+} and b_j are Boson operators satisfying the Boson commutative relation. Applying the transformations (3*a*) and (3*b*) to the Hamiltonian $H_{\parallel}$ and using the operator expressions (4*a*) and (4*b*) 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 SO phonon, we can easily obtain

$$\mathcal{H}_{\parallel} = U_2^{-1}U_1^{-1}H_{\parallel}U_1U_2 = \mathcal{H}_{\parallel}^0 + \mathcal{H}_{\parallel}' \tag{5a}$$

$$\begin{aligned}\mathcal{H}_{\parallel}^0 = {} & \frac{\lambda}{2}\Big(\sum_j b_j^+ b_j + 1\Big) + \frac{\lambda}{4}\sum_j (b_j^+ b_j^+ + b_j b_j + P_{0j}^2) + \frac{\lambda}{2}\sum_j (b_j^+ + b_j)P_{0j} \\ & + \sum_{\boldsymbol{W}} \omega_l (a_{\boldsymbol{W}}^+ + f_W^*)(a_{\boldsymbol{W}} + f_W) + \sum_{\boldsymbol{Q}} \omega_s (b_{\boldsymbol{Q}}^+ + g_Q^*)(b_{\boldsymbol{Q}} + g_Q) \\ & + \frac{1}{2}\Big(\sum_{\boldsymbol{W}} \boldsymbol{W}_{\parallel}(a_{\boldsymbol{W}}^+ + f_W^*)(a_{\boldsymbol{W}} + f_W)\Big)^2 - \Big(\frac{\lambda}{2}\Big)^{\frac{1}{2}} \sum_{\boldsymbol{W}} (a_{\boldsymbol{W}}^+ + f_W^*)(a_{\boldsymbol{W}} + f_W) \\ & \times \sum_j (b_j^+ + b_j + P_{0j}) + \sum_{\boldsymbol{W}} \sin(W_z z)(V_W^*(a_{\boldsymbol{W}}^+ + f_W^*) + \mathrm{HC}) \\ & + \sum_{\boldsymbol{Q}} \mathrm{e}^{-Qz}\,(V_Q^*(b_{\boldsymbol{Q}}^+ + g_Q^*))\,\mathrm{e}^{-(Q^z/4\lambda)} \\ & \times \mathrm{e}^{-(1/2\lambda)^{\frac{1}{2}}\sum_j b_j^+ Q_j}\,\mathrm{e}^{(1/2\lambda)^{\frac{1}{2}}\sum_j b_j Q_j} + \mathrm{HC})\end{aligned} \tag{5b}$$

$$\mathcal{H}_{\parallel}' = \frac{1}{2}\sum_{\boldsymbol{W}\neq\boldsymbol{W}'} \boldsymbol{W}_{\parallel}\cdot\boldsymbol{W}_{\parallel}'(a_{\boldsymbol{W}'}^+ + f_W^*)(a_{\boldsymbol{W}} + f_W)(a_{\boldsymbol{W}'}^+ + f_{W'}^*)(a_{\boldsymbol{W}'} + f_{W'}). \tag{5c}$$

(5*c*) is the term describing the interaction between phonons of different wave vectors in the recoil process. The ground-state wavefunction of the system is $\phi = \varphi(\rho)|0\rangle$ where $\varphi(\rho)$ is the normalized surface polaron wavefunction. $|0\rangle$ is the zero-phonon state, which satisfies

$$a_{\boldsymbol{W}}|0\rangle = b_{\boldsymbol{Q}}|0\rangle = b_j|0\rangle = 0. \tag{6}$$

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 quasi-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;

$$\boldsymbol{P}_{\parallel T} = \boldsymbol{P}_{\parallel} + \sum_{\boldsymbol{W}} \boldsymbol{W}_{\parallel}^+ a_{\boldsymbol{W}}^+ a_{\boldsymbol{W}} + \sum_{\boldsymbol{Q}} \boldsymbol{Q} b_{\boldsymbol{Q}}^+ b_{\boldsymbol{Q}}. \tag{7}$$

The minimization problem is now carried out by the use of the Lagrange multiplier $\boldsymbol{u}$; we have

$$\langle\phi|\boldsymbol{H}_{\parallel}^0 - U_2^{-1}U_1^{-1}\boldsymbol{u}\cdot\boldsymbol{P}_{\parallel T}U_1U_2|\phi\rangle = \langle\varphi(\rho)|F(\lambda, f_W, g_Q, u, p_0)|\varphi(\rho)\rangle \tag{8a}$$

where

$$\begin{aligned}F(\lambda, f_W, g_Q, u, P_0) = {} & \langle 0|\mathcal{H}_{\parallel}^0 - U_2^{-1}U_1^{-1}\boldsymbol{u}\cdot\boldsymbol{P}_{\parallel T}U_1U_2|0\rangle = \frac{\lambda}{2} + \frac{\lambda}{4}p_0^2 + \sum_W \omega_l |f_W|^2 \\ & + \sum_Q \omega_s |g_Q|^2 + \frac{1}{2}\Big(\sum_W |f_W|^2 \boldsymbol{W}_{\parallel}\Big)^2 + \frac{1}{2}\sum_W |f_W|^2 W_{\parallel}^2 \\ & - \Big(\frac{\lambda}{2}\Big)^{\frac{1}{2}} \sum_W |f_W|^2 \boldsymbol{p}_0\cdot\boldsymbol{W}_{\parallel} + \sum_W \sin(w_z z)(V_W^* f_W^* + V_W f_W) \\ & + \sum_Q \mathrm{e}^{-Qz}(V_Q^* g_Q^* + V_Q g_Q)\,\mathrm{e}^{-(Q^2/4\lambda)} - \Big(\frac{\lambda}{2}\Big)^{\frac{1}{2}} \boldsymbol{p}_0\cdot\boldsymbol{u} - \sum_Q \boldsymbol{Q}\cdot\boldsymbol{u}|g_Q|^2\end{aligned} \tag{8b}$$

$F(\lambda, f_W, g_Q, u, p_0)$ may be called the variational parameter function. Minimizing (8*b*) with respect to λ, f_W, g_Q, u and p_0, we can determine these parameters and functions. Using the variational method, we obtain

$$f_W = -\frac{V_W^* \sin(W_z z)}{\omega_l + W_\parallel^2/2 - ((\lambda/2)^{1/2} - \eta)\boldsymbol{p}_0 \cdot \boldsymbol{W}_\parallel} \tag{9a}$$

$$g_Q = -\frac{\mathrm{e}^{-Qz} V_Q^* \, \mathrm{e}^{-(Q^2/4\lambda)}}{\omega_s \boldsymbol{Q} \cdot \boldsymbol{u}}. \tag{9b}$$

According to the Lee–Low–Pines [17] variation technique, if it is noted that the only preferred direction in the x–y plane is that of $\boldsymbol{p}_0$, we may conveniently introduce the parameter defined by

$$\sum_W |f_W|^2 \boldsymbol{W}_\parallel = \eta \boldsymbol{p}_0. \tag{10}$$

Substituting (9*a*) into (10), we obtain

$$\eta = \frac{2\alpha_l f_1(z)}{1 + 2\alpha_l f_1(z)} \left(\frac{\lambda}{2}\right)^{\frac{1}{2}} \tag{11a}$$

$$f_1(z) = \frac{\pi}{8} - 2\int_0^\infty \frac{x^2 e^{-2u_l z x}}{(1+x^2)^3} \, \mathrm{d}x. \tag{11b}$$

Substituting (9) into (8*b*), the final two terms in (8*b*) 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 $\boldsymbol{p}_0 \cdot \boldsymbol{W}_\parallel$ and $\boldsymbol{Q} \cdot \boldsymbol{u}$ are equal to zero; thus, we have

$$\begin{aligned} F(\lambda, u, p_0) = {} & \frac{\lambda}{2} + \frac{\lambda}{4} p_0^2 - \left(\frac{\lambda}{2}\right)^{\frac{1}{2}} \boldsymbol{p}_0 \cdot \boldsymbol{u} - \alpha_l \omega_l f_2(z) - \alpha_l p_0^2 \left(\lambda - 3\left(\frac{\lambda}{2}\right)^{\frac{1}{2}} \eta + \eta^2\right) f_1(z) \\ & + \frac{\alpha_l^2 p_0^2}{2} \left(\left(\frac{\lambda}{2}\right)^{\frac{1}{2}} - \eta\right)^2 f_1^2(z) - \alpha_s \omega_s \left(\frac{\lambda}{\omega_s}\right)^{\frac{1}{2}} \int_0^\infty \mathrm{e}^{-x^2 - 2u_\lambda z x} \, \mathrm{d}x \\ & - \alpha_s u^2 \left(\frac{\lambda}{\omega_s}\right)^{\frac{3}{2}} \int_0^\infty x^2 \, \mathrm{e}^{-x^2 - 2u_\lambda z x} \, \mathrm{d}x \end{aligned} \tag{12a}$$

where

$$f_2(z) = \frac{\pi}{2} - \int_0^\infty \frac{\mathrm{e}^{2u_l z x}}{1 + x^2} \, \mathrm{d}x \tag{12b}$$

$$\alpha_l = \frac{e^2}{\varepsilon u_l} \qquad \alpha_s = \frac{e^2}{\varepsilon^* u_s} \tag{12c}$$

$$u_l = (2\omega_l)^{\frac{1}{2}} \qquad u_s = (2\omega_s)^{\frac{1}{2}} \qquad u_\lambda = (2\lambda)^{\frac{1}{2}}. \tag{12d}$$

The extremum condition $\partial F / \partial p_0 = 0$ given by

$$\boldsymbol{p}_0 = \left(\frac{2}{\lambda}\right)^{\frac{1}{2}} \frac{(1 + 2\alpha_l f_1(z))^2}{1 + 3\alpha_l f_1(z) + \alpha_l^2 f_1^2(z)} \boldsymbol{u} \tag{13a}$$

$$\langle 0 | \boldsymbol{u} \cdot \boldsymbol{p}_0 | 0 \rangle = 2\alpha_s u^2 \left(\frac{\lambda}{\omega_s}\right)^{\frac{3}{2}} \int_0^\infty x^2 \, \mathrm{e}^{-x^2 - 2u_\lambda z x} \, \mathrm{d}x + u^2 \left\{ \frac{(1 + 2\alpha_l f_1(z))^2}{1 + 3\alpha_l f_1(z) + \alpha_l^2 f_1^2(z)} \right\}. \tag{13b}$$

Finally, the Hamiltonian of the surface polaron in a plane parallel to the surface, which omits the interaction between phonons of different wave vectors in the recoil process, can be expressed as

$$\mathcal{H}_{\parallel}^{0} = F(\lambda, u) - \langle 0|\boldsymbol{u}\cdot\boldsymbol{p}_0|0\rangle = \frac{\lambda}{2} + \frac{p_{\parallel}^2}{2m^*} - \alpha_l\omega_l f_2(z) + \alpha_s\omega_s\left(\frac{\lambda}{\omega_s}\right)^{\frac{1}{2}}\int_0^{\infty} \mathrm{e}^{-x^2-2u_\lambda zx}\,\mathrm{d}x \tag{14a}$$

where

$$m^* = \frac{(1+2\alpha_l f_1(z))^2}{1+3\alpha_l f_1(z)+\alpha_l^2 f_1^2(z)} + 2\alpha_s\left(\frac{\lambda}{\omega_s}\right)^{\frac{3}{2}}\int_0^{\infty} x^2\,\mathrm{e}^{-x^2-2u_\lambda zx}\,\mathrm{d}x \tag{14b}$$

is the effective mass of the surface polaron, which omits the corresponding interaction. Performing the variation of $\mathcal{H}_{\parallel}^{0}$ with respect to λ, we obtain

$$\lambda^{1/2} = \alpha_s\sqrt{\omega}_s\int_0^{\infty}(1-2u_\lambda zx)\,\mathrm{e}^{-x^{-2}-2u_\lambda zx}\,\mathrm{d}x. \tag{15}$$

3. Perturbation calculation

We regard $\mathcal{H}_{\parallel}^{0}$ as the unperturbed Hamiltonian of the surface polaron–phonon system, and $\mathcal{H}_{\parallel}'$ as the perturbation part in the perturbation calculation. The first-order perturbation energy induced by $\mathcal{H}_{\parallel}'$ is zero. Now we are ready to calculate the second-order perturbation energy,

$$\Delta E' = -{\sum_n}' \frac{|(\mathcal{H}_{\parallel}')_{0n}|^2}{E_n - E_0} = -\alpha_l^2\omega_l f_3(z) - \frac{u^2(1+2\alpha_l f_1(z))^2\alpha_l^2}{2(1+3\alpha_l f_1(z)+\alpha_l^2 f_1^2(z))^2}(3f_4(z)+f_5(z)) \tag{16a}$$

$$f_3(z) = \frac{1}{2}\int_0^{\infty}\int_0^{\infty}\frac{x^2y^2(1-\mathrm{e}^{-2u_lzx})(1-\mathrm{e}^{-2u_lzy})}{(1+x^2)^2(1+y^2)^2(2+x^2+y^2)}\,\mathrm{d}x\,\mathrm{d}y \tag{16b}$$

$$f_4(z) = \int_0^{\infty}\int_0^{\infty}\frac{x^4y^2(1-\mathrm{e}^{-2u_lzx})(1-\mathrm{e}^{-2u_lzy})}{(1+x^2)^4(1+y^2)^2(2+x^2+y^2)}\,\mathrm{d}x\,\mathrm{d}y \tag{16c}$$

$$f_5(z) = \int_0^{\infty}\int_0^{\infty}\frac{x^4y^2(1-\mathrm{e}^{-2u_lzx})(1-\mathrm{e}^{-2u_lzy})}{(1+x^2)^2(1+y^2)^2(1+x^2+y^2)^3}\,\mathrm{d}x\,\mathrm{d}y. \tag{16d}$$

In (16*a*), the first term, being proportional to the squared coupling constant α_l^2, is the extra energy of the induced potential of the surface polaron, considering interaction between phonons of different wave vectors in the recoil process. The second term, being proportional to the squared coupling constant α_l^2, is the extra effective mass of the surface polaron, considering the corresponding interaction. Finally, the effective Hamiltonian of the surface polaron can be expressed as

$$\mathcal{H}_{eff} = H_z + \mathcal{H}_{\parallel}^{0} + \Delta E' = \frac{P_z^2}{2} + \frac{P_{\parallel}^2}{2m^*} + \frac{\lambda}{2} + V_{img} + V_i^b + V_i^s \tag{17a}$$

where

$$V_{img} = \frac{e^2(\varepsilon_\infty - 1)}{4z\varepsilon_\infty(\varepsilon_\infty - 1)} \tag{17b}$$

$$V_i^b = -\alpha_l\omega_l f_2(z) - \alpha_l^2\omega_l f_3(z) \tag{17c}$$

$$V_i^s = \alpha_s\omega_s\left(\frac{\lambda}{\omega_s}\right)^{\frac{1}{2}}\int_0^\infty \mathrm{e}^{-x^2-2u_\lambda zx}\,\mathrm{d}x \tag{17d}$$

$$m^* = \frac{(1+2\alpha_l f_1(z))^2}{1+3\alpha_l f_1(z)+\alpha_l^2 f_1^2(z)}\left(1-\frac{\alpha_l^2(3f_4(z)+f_5(z)}{1+3\alpha_l f_1(z)+\alpha_l^2 f_1^2(z)}\right) + 2\alpha_s\left(\frac{\lambda}{\omega_s}\right)^{\frac{3}{2}}\int_0^\infty x^2\,\mathrm{e}^{-x^2-2u_\lambda zx}\,\mathrm{d}x \tag{17e}$$

are the image potential, the potential induced by the electron–LO phonon interaction, the potential induced by the electron–SO phonon interaction and the effective mass of the surface polaron, respectively. The effective interaction potential of the surface polaron is defined as

$$V_{eff} = V_{img} + V_i^b + V_i^s. \tag{17f}$$

Evidently, the induced potential V_i^b, the effective mass m^* and the effective interaction potential V_{eff} of the surface polaron depend on the interaction between phonons of different wave vectors in the recoil process.

4. Results and discussion

To show more obviously the influence of the interaction between phonons of different wave vectors in the recoil process on the properties of the surface polaron, taking the polaron in the surface of an AgBr crystal as an example, we perform a numerical evaluation. In table 1, the data for an AgBr crystal are given.

Table 1. The data for an AgBr crystal. All the parameters are taken from [18].

Material	ε_0	ε_∞	$\hbar\omega_l$ (meV)	$\hbar\omega_s$ (meV)	α_l	α_s	u_l (cm^{-1})	u_s (cm^{-1})
AgBr	10.6	4.68	17.1	14.5	1.56	2.56	311.5×10^4	286.8×10^4

Figure 1 shows the relationships 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 interaction potential V_{eff} of the surface polaron in the AgBr crystal, considering the corresponding interactions, and the coordinate z. From figure 1 one can see that the induced potential V_i^s of the surface polaron will decrease with increasing coordinate z, whereas the induced potential V_i^b of the surface polaron will increase with increasing coordinate z. Near the surface the electron–SO phonon interaction is dominant, whereas in the bulk far from the surface the electron–bulk LO phonon interaction is dominant. As $z \to 0$, the first term of (17*f*) is dominant, and the surface polaron will be repulsed away from the surface. Thus the surface polaron cannot approach infinitely close to the surface; there is no surface polaron in the range near the

surface ($V_{eff} > 0$). 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

$$V_{eff}(z) = 0 \tag{18}$$

the root is the depth of the SPFSL, which we denote as d (for the AgBr crystal, $d = 10.67$ Å).

This shows that, when the distance between the electron and the surface is much smaller than the radius of the bulk polaron the effect of the bulk phonons can be neglected, and so can the effect of the surface phonons when the corresponding distance is much larger than the corresponding radius.

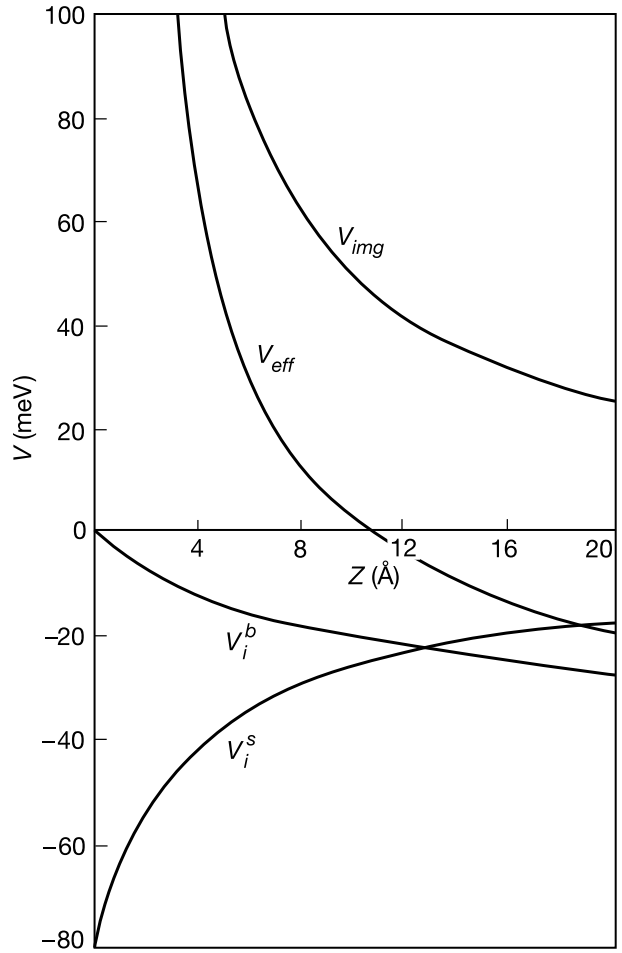

Figure 1. The relational curves of V_{img}, V_i^s, V_i^b and V_{eff} with coordinate z.

In general, as the distance between the electron and the surface is of the same order of magnitude as the radius of the bulk polaron, the effects of both the bulk LO and the SO phonons must be taken into account. In this case the electron moves in a non-local potential as given by (17*a*) [7].

The effective mass m^* of the surface polaron can be expressed as

$$m^* = m_b^* + m_s^* \tag{19a}$$

where

$$m_b^* = \frac{(1+2\alpha_l f_1(z))^2}{1+3\alpha_l f_1(z)+\alpha_l^2 f_1^2(z)} - \frac{\alpha_l^2(1+2\alpha_l f_1(z))^2(3f_4(z)+f_5(z))}{(1+3\alpha_l f_1(z)+\alpha_l^2 f_1^2(z))^2} \tag{19b}$$

$$m_s^* = 2\alpha_s\left(\frac{\lambda}{\omega_s}\right)^{\frac{3}{2}}\int_0^\infty x^2\,\mathrm{e}^{-x^2-2u_\lambda zx}\,\mathrm{d}x \tag{19c}$$

are the effective mass induced by the electron–bulk LO phonon interaction and by the electron–SO phonon interaction, respectively. Figure 2 gives the relationship between the effective masses of the surface polaron m^*, m_b^* and m_s^* in an AgBr crystal with the coordinate z. From the figure one can see that the effective mass m_b^* induced by the electron–bulk LO phonon interaction will increase little with increasing coordinate z, whereas the effective mass m_s^* induced by the electron–SO phonon interaction and the effective mass m^* of the surface polaron will increase strongly with decreasing coordinate z.

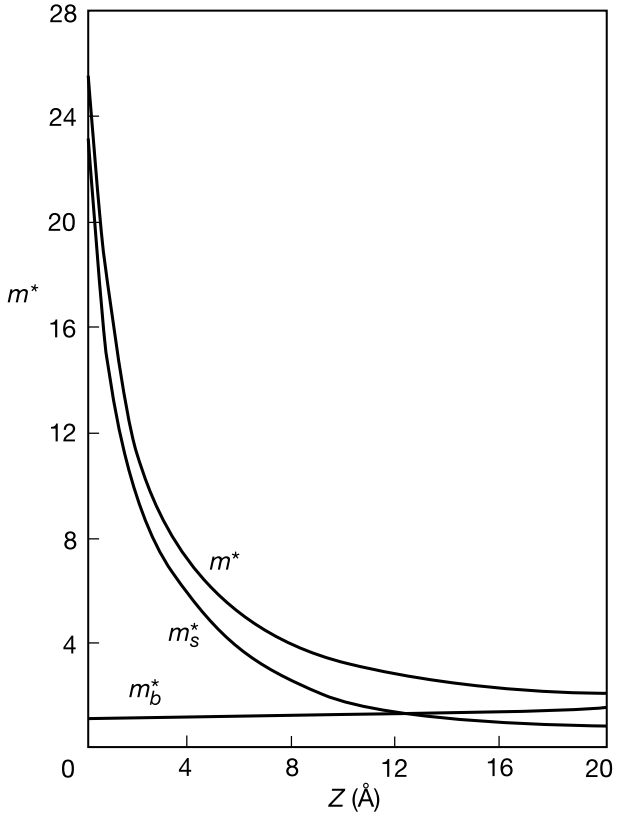

Figure 2. The relational curve of m^* with coordinate z in the AgBr crystal.

Since there is weak bulk but strong surface coupling between electrons and phonons in polar crystals, the interaction between phonons of different wave vectors in the recoil process influences only the induced potential V_i^b and the effective mass m_b^* resulting from

the electron–bulk LO phonon interaction. The extra induced potential, considering the interaction between phonons of different wave vectors in the recoil process, is given by

$$V_{i2}^{b} = \alpha_l^2 \omega_l f_3(z). \tag{20a}$$

The induced potential, omitting the corresponding interaction, is

$$V_{i1}^{b} = \alpha_l^2 \omega_l f_2(z). \tag{20b}$$

The ratio of V_{i2}^{b} and V_{i1}^{b} is

$$\Delta_1 = \frac{V_{i2}^{b}}{V_{i1}^{b}} = \alpha_l \frac{f_3(z)}{f_2(z)}. \tag{20c}$$

The extra effective mass, considering the corresponding interaction, is given by

$$m_{b2}^{*} = \frac{\alpha_l^2 (1 + 2\alpha_l f_1(z))^2 (3 f_4(z) + f_5(z))}{(1 + 3\alpha_l f_1(z) + \alpha_l^2 f_1^2(z))^2}. \tag{21a}$$

The effective mass, omitting the corresponding interaction, is

$$m_{b1}^{*} = \frac{(1 + 2\alpha_l f_1(z))^2}{1 + 3\alpha_l f_1(z) + \alpha_l^2 f_1^2(z)}. \tag{21b}$$

The ratio of m_{b2}^{*} and m_{b1}^{*} is

$$\Delta_2 = \frac{m_{b2}^{*}}{m_{b1}^{*}} = \frac{\alpha_l^2 (3 f_4(z) + f_5(z))}{(1 + 3\alpha_l f_1(z) + \alpha_l^2 f_1^2(z))^2}. \tag{21c}$$

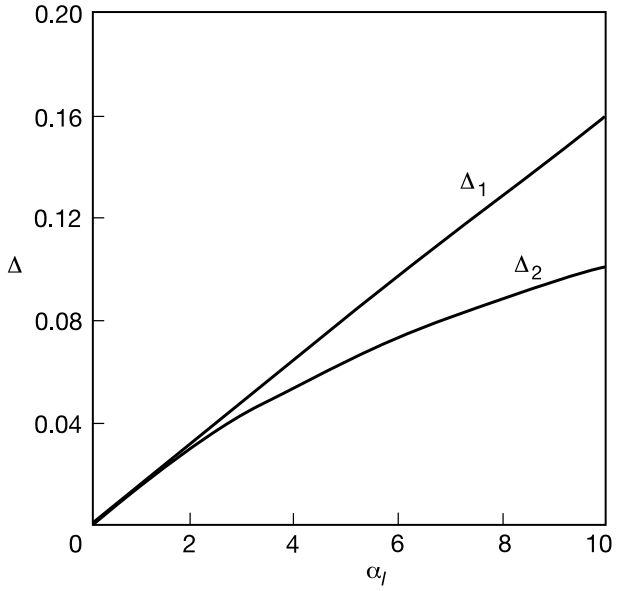

Figure 3. The relational curve of Δ_1 and Δ_2 with coupling constant α_l.

Figure 3 gives a description of the variation of Δ_1 and Δ_2 with coupling constant α_l: Δ_1 and Δ_2 increase with increasing coupling constant α_l. For example, when $\alpha_l = 3$ and 6, the ratio of the extra induced potential, considering the corresponding interaction, to the induced potential, omitting the corresponding interaction, is $\Delta_1 = 4.8\%$ and 9.6%; the

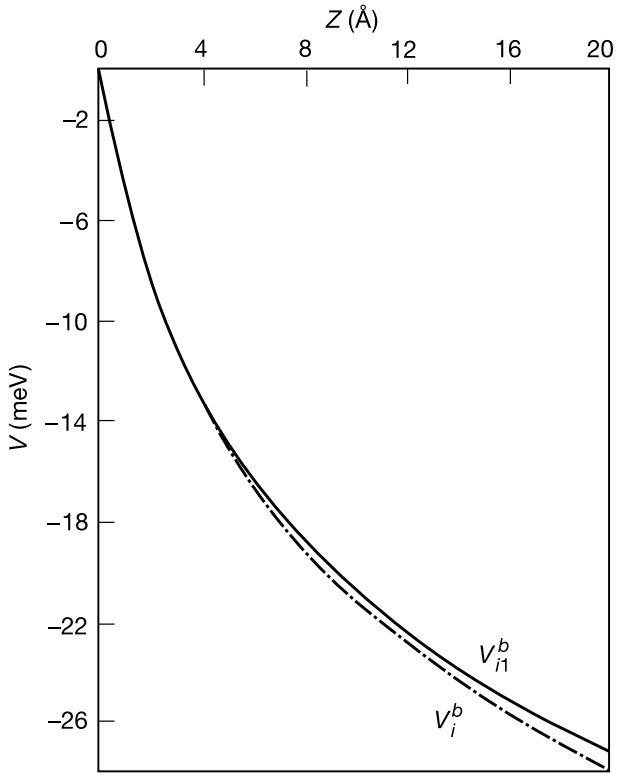

Figure 4. The relational curve of V_{i1}^b and V_i^b with coordinate z for the AgBr crystal.

ratio of the extra effective mass, considering the corresponding interaction, and the effective mass, omitting the corresponding interaction, is $\Delta_2 = 4.2\%$ and 7.2%.

Figure 4 shows the relationship between the induced potential V_{i1}^b, omitting the corresponding interaction, and the induced potential V_i^b, considering the corresponding interaction, and the coordinate z. The solid curve denotes the case of V_{i1}^b; the dashed one represents the case of V_i^b. From the figure, one can see that the induced potential V_{i1}^b and V_i^b will increase with increasing coordinate z; moreover, V_i^b will increase more than V_{i1}^b with increasing coordinate z. Figure 5 shows the variation of the effective mass m_b^*, considering the corresponding interaction, and the effective mass m_{b1}^*, omitting the corresponding interaction, with the coordinate z. The solid curve denotes the case of m_{b1}^*; the dashed one represents the case of m_b^*. It can be seen from figure 5 that the effective masses m_{b1}^* and m_b^* will decrease with increasing coordinate z; moreover, m_b^* will decrease more than m_{b1}^* with increasing coordinate z.

5. Conclusion

Taking into account the interaction of an electron with both the weak-coupling bulk LO and the strong-coupling SO phonons we use an improved linear combination operator and perturbation methods to study the influence of the interaction between phonons of different wave vectors in the recoil process on the properties of the surface polaron in a semi-infinite

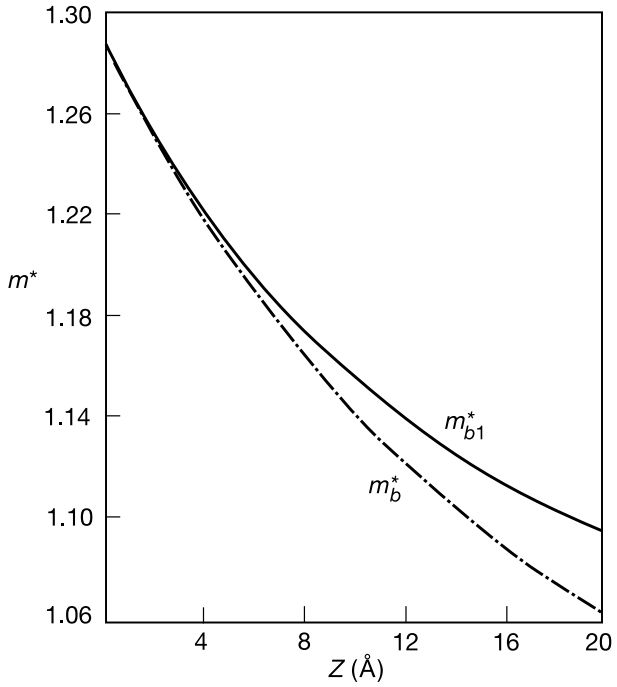

Figure 5. The relational curve of m^*_{b1} and m^*_b to coordinate z for the AgBr crystal.

crystal. Numerical calculations, taking the AgBr crystal as an example, are performed. The results show that the influence of the corresponding interaction on the induced potential and effective mass will increase with increasing coupling constant α_l, and the influence on the induced potential will increase more with increasing coordinate z, and the influence on the effective mass will decrease more with increasing z.

Acknowledgment

One of us (J L Xiao) wishes to acknowledge support by the National Science Foundation of Inner Mongolia.

References

[1] Ibach H 1970 *Phys. Rev. Lett.* **24** 141
Ibach H 1971 *Phys. Rev. Lett.* **27** 253
[2] Lucas A A, Kartheuser E and Badro R G 1970 *Phys. Rev.* B **2** 2485
[3] Pan J S 1985 *Phys. Status Solidi* b **127** 307
Pan J S 1985 *Phys. Status Solidi* b **128** 287
[4] Xiao J L, Sun B Q and Xiao W 1993 *Phys. Status Solidi* b **176** 117
[5] Evans E and Mills L 1972 *Solid State Commun.* **11** 1093
Evans E and Mills L 1973 *Phys. Rev.* B **8** 4004
[6] Gu S W and Yan G 1982 *J. Semicond.* **3** 426 (in Chinese)
[7] Liang X X and Gu S W 1984 *Solid State Commun.* **50** 505

[8] Huybrechts J 1976 *J. Phys. C: Solid State Phys.* **9** L211
[9] Gu S W and Zheng J 1984 *Phys. Status Solidi* b **121** K165
[10] Tokuda N 1980 *J. Phys. C: Solid State Phys.* **13** L173
[11] Sun B Q, Xiao W and Xiao J L 1994 *J. Phys.: Condens. Matter* **6** 8167
[12] Tokuda N 1980 *J. Phys. C: Solid State Phys.* **13** L851
[13] Xiao J L, Xing T H, Sun B Q and Xiao W 1994 *Phys. Status Solidi* b **183** 425
[14] Haga E 1954 *Prog. Theor. Phys.* **11** 449
[15] Wei B H and Gu S W 1991 *Phys. Rev.* B **43** 9190
[16] Wei B H, Liu Y Y, Gu S W and Yu W K 1992 *Phys. Rev.* B **46** 4269
[17] Lee T D, Low F E and Pines D 1953 *Phys. Rev.* **90** 297
[18] Kartheuser E 1972 *Polarons in Ionic Crystals and Polar Semiconductors* (Amsterdam: North-Holland)