Two-dimensional image-potential-induced electron band

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Image states represent a simple type of surface state which is very useful for studying the two-dimensional (2D) electron gas. In liquid helium an instability of the 2D electron gas develops when the density is increased. In metals the intraband and interband energy half-widths of the state are comparable (a few meV), thus preventing a steady-state population of these states. Insulators could provide a good compromise between these two extreme cases. The lifetime of electrons in a 2D electron band at a vacuum-insulator interface is studied in this paper.

Image states represent a very simple and fundamental class of surface state which is useful in studying the two-dimensional (2D) electron gas.[1] Two dimensional means that the components of the system (electrons) are essentially free to move in two spatial dimensions but their motion is constrained in the third dimension. The energy levels take the form (atomic units are used throughout this paper except where explicitly expressed)

$$E=E_n+\frac{k_x^2+k_y^2}{2}\ ,$$

where k_x and k_y are the momentum components of the motion parallel to the surface and E_n are the levels in the potential well for the normal motion. Each value of E_n is the bottom of a 2D continuum band. Intensive work has been done to understand the properties of image states of different surfaces.[2]

To obtain a 2D Fermi electron gas a high-electron density is needed. In liquid helium[3] the binding energy is weak ($\approx$meV) and an instability of the 2D electron gas develops when the density is increased.[4] In metals[5] the binding energy is of the order of 1 eV but a problem arises due to the processes that contribute to the energy width of the image state. These processes are the decay into allowed bulk states (interband transition) and the decay into image states having smaller parallel momentum within the band (intraband transition). The interband transition contribution to the energy width is *high* and *comparable to* the intraband contribution.[6] This means that electrons may not be able to thermalize to the bottom of the 2D band because they would leave it before by decaying into bulk states and the high density needed would not be achieved. Other materials with a relatively strong binding energy and small interband energy width might be better candidates to build a 2D Fermi electron gas. In insulators, such as diamond or LiF, relatively strong binding appears (a big enough dielectric constant) and the escape outside the band into bulk states is prevented by the electronic structure.

The electronic structure of LiF exhibits[7,8] a band gap of about 13–14 eV and the position of the bottom of the conduction band is about 2–4 eV above the vacuum level. The binding energy of the first image state is a few tenths of eV,[7] so that we can neglect the wave function penetration into the bulk, and there are no empty states in the bulk to decay into. This means that the only significant contribution to the energy width of the states comes from the loss of parallel momentum within the band (intraband transition). For high parallel momentum there is also a small contribution to the energy width from processes in which there is a transition from an image state in the first band of normal motion to another image state in a higher band with smaller parallel momentum (interband transition). In these conditions (the intraband half-width of the state is much greater than the interband half-width of the state $\cong 0$) it is possible to think of filling a 2D electron band. The remaining problem should be the experimental procedure to fill these states efficiently.

In this paper we calculate the energy half-width of the first image state of an electron at a vacuum-LiF surface using a self-energy formalism. The self-energy of the electron is calculated using a GW approximation.[9] For LiF we approximate the long-wavelength response by the schematic dielectric function:[10]

$$\epsilon(\omega)=1+\frac{\Omega_e^2}{\omega_e^2-\omega(\omega+i\gamma)}+\frac{\Omega_t^2}{\omega_t^2-\omega(\omega+i\gamma)}\quad(\gamma\rightarrow 0)\ . \tag{1}$$

In Eq. (1) ω_t is the frequency of the transverse optical phonons and ω_e is an effective energy of electronic transitions, $\Omega_e^2=4\pi n\alpha_0\omega_e^2$ where n is the atomic density and α_0 is the static atomic polarizability and $\Omega_t^2=\omega_l^2-\omega_t^2$, where ω_l is the longitudinal optical-phonon frequency. If ϵ_0 is the static dielectric constant and ϵ_∞ is the dielectric constant for frequencies $\omega_t \ll \omega \ll \omega_e$, the following relations hold:

$$\epsilon_0=1+\frac{\Omega_e^2}{\omega_e^2}+\frac{\Omega_t^2}{\omega_t^2}\quad\text{and}\quad\epsilon_\infty=1+\frac{\Omega_t^2}{\omega_t^2}\ .$$

For LiF the following parameters have been used: $\omega_t=38$ meV, $\omega_e=16.8$ eV, $\epsilon_0=8.65$, and $\epsilon_\infty=1.92$. A medium described by this response function will support two different surface modes; surface optical phonons with frequency

$$\omega_S=\omega_T\left[\frac{1+\epsilon_0}{1+\epsilon_\infty}\right]^{1/2}$$

and surface excitons (SE)[11] with frequency

$$\omega_{\mathrm{SE}}=\omega_e\left[\frac{1+\epsilon_\infty}{2}\right]^{1/2} .$$

The energy half-width of the state with finite parallel momentum, k_p, calculated from the imaginary part of the self-energy is given by

$$\frac{\Gamma}{2}=\frac{\omega_s}{2}(A_0-A_\infty)\sum_n\int_{Q_-}^{Q_+}dQ\frac{|\langle 0|e^{-Qz}|n\rangle|^2}{[(k_pQ)^2-(\omega_S+\frac{1}{2}Q^2+E_n-E_0)^2]^{1/2}}\Theta(k_p^2-2(\omega_S+E_n-E_0)) , \tag{2}$$

where

$$Q_{+(-)}=k_p+(-)[k_p^2-2(\omega_s+E_n-E_0)]^{1/2} ,$$

$$A_{0(\infty)}=\frac{\epsilon_{0(\infty)}-1}{\epsilon_{0(\infty)}+1} .$$

$\Theta(x)$ is the unit step function and $|n\rangle$ are the states describing the perpendicular motion with energies E_n. It is interesting to note that the surface exciton does not contribute to the energy half-width of the state at the energies we are interested. The main contribution to the energy half-width comes from the first term ($n=0$) but we have calculated also the second term ($n=1$). The binding energy of the first image state has been calculated variationally[12] using a hydrogenic trial wave function.[13] We stress the importance of a variational calculation of the binding energy since in this case (small ω_S compared with the plasmon energy in metals) the classical approximation to the image potential is not a good one in the region where the image state lies. This can be easily seen if we approximate the image potential by[14]

$$V(z)=-\frac{Z_s}{4z}(1-e^{-\lambda_s z})-\frac{Z_e}{4z}(1-e^{-\lambda_e z}) , \tag{3}$$

where

$$Z_s=A_0-A_\infty,\quad Z_e=A_\infty ,$$

$$\lambda_s=\pi(2\omega_S)^{1/2},\quad \lambda_e=\pi(2\omega_{\mathrm{SE}})^{1/2} .$$

These parameters are obtained by fixing the correct asymptote of the image potential and the saturation value at $z=0$ from the real part of the self-energy. The variational calculation using the real part of the self-energy gives $E_0=-0.29$ eV and with the model potential of Eq. (3) we obtain $E_0=-0.34$ eV. If we had used the classical approximation to the image potential we should have obtained $E_0=-0.53$ eV. The results obtained for the energy half-width of the first image state are shown in Table I. $\Gamma^{00}/2$ is obtained from the first term ($n=0$) in Eq. (2) and $\Gamma^{01}/2$ is obtain from the second. $\Gamma^{00}/2$ represents the contribution to the energy half-width of the state from transitions without change of state in the perpendicular motion (intraband). The minimum parallel momentum required for this transition is $k_{p0}=(2\omega_S)^{1/2}$ and it is about 0.13 Å^{-1}. $\Gamma^{01}/2$ represents the contribution from transitions in which the energy of the parallel motion of the initial state in the lower band allows a final state in the next 2D band with smaller parallel momentum together with the excitation of a surface optical phonon (interband). The contribution to the energy half-width of the first state from transitions with change of state in the perpendicular motion (interband) is much smaller because these transitions are energetically less favorable. For example, the minimum parallel momentum, $k_{p01}=[2(\omega_S+E_1-E_0)]^{1/2}$, required for the $|0\rangle\rightarrow|1\rangle$ transition is about 0.25 Å^{-1}. The results obtained show that if we could populate the first image-state electron band until $k_p=0.13$ Å^{-1} we should have a density of about 10^{13} cm^{-2}, enough to think in terms of a 2D Fermi electron gas.[15]

TABLE I. Energy half-widths of the first image state (in meV) for different values of the parallel momentum k_p (in Å^{-1}). $\Gamma^{00}/2$ is obtained from the first term ($n=0$) in Eq. (2) and $\Gamma^{01}/2$ from the second ($n=1$).

k_p (Å^{-1})	$\Gamma^{00}/2$ (meV)	$\Gamma^{01}/2$ (meV)
0.15	153	0
0.19	147	0
0.28	132	0.39
0.38	119	1.21
0.57	99	1.32
0.76	85	1.27

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