Ground- and Excited-State Impurity Bands in Silicon Inversion Layers

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Impurities in silicon inversion layers have been the subject of considerable experimental and theoretical iiiterest. Tlie main purpose of tliis investigation is to extencl the recent work on ground charged impurities n-type Si inversion layers to tlie case of the lowest excited states. We show that, with the effects of disorder and for given impurity concentrations, binding energies and electric fields of interest, tlie lowest excited band would play an essential role in tlie optical and transport measurements.

I. Theory

Tlieoretical investigations of tlie grountl- and excited- statr impurity bands in inversion layers of metal-oxide-semiconductor (MOS) structures are important for tlie design and the interpretation of experiments[1,2].

In wake cf a. recent work[1], we present a thorough analysis of tlie ground and excited states in these structures.

Tlie system can be described by the Hamiltonian

$$H = E_\lambda^B \sum_i a_i^+ a_i + \sum_{i \neq j} V_{ij} a_i^+ a_j \ , \qquad (1)$$

where the creation annihilation operator a_i^+ (a_i) describes an electron bound to tlie ground (excited) state of a single impurity at site i. E_λ^B is tlie binding energy, which is taken as our reference energy below tlie edge of the unperturbed first conduction band (UFCB), λ are the states to be considered, and V_{ij} is tlie hopping energy integral.

The states are described by the wave functions[1]

$$\psi_\lambda(\vec{R}z) = \phi_\lambda(\vec{R})\varphi(z) \ , \qquad (2)$$

where $\vec{R} = \vec{R}(x,y)$, and

$$\phi_{2p_o}(R) = (a_0^2/2\pi)^{1/2} \exp(-a_0 R/2) \qquad (3)$$

represents the surface ground state,

$$\phi_{3d\pm1}(R) = (a_1^4/12\pi)^{1/2}(x \pm iy)\exp(-a_1 R) \ , \qquad (4)$$

represents tlie lowest excited state, and

$$\varphi(z) = (b^3/2)^{1/2} \exp(-bz) \qquad (5)$$

is the lowest electric subband. The variational parameters a_0, a_1 and b will be determined by ininimizing the value of tlie Hamiltonian, calculating the energies

$$E_\lambda = < \psi_\lambda(R,z)|-\nabla_R^2 - \nu\nabla_z^2 + \frac{\delta}{z} + \epsilon z - 2\Phi(\vec{r})|\psi_\lambda(R,z) > \qquad (6)$$

In tliis equation ϵ is the externa1 electric field, $\Phi(\vec{r})$, $\vec{r} = \vec{r}(x,y,t)$, is the screened Coulomb potential energy $\Phi(r) = \Phi(\vec{r},s,z_0)$[1-3] produced by tlie impurity

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within the oxide on the inversion layer electron, s is the screening parameter, aiid z_0 is the distance between tlie externa1 charged and the $S_i - S_iO_2$ interface. $\mathbf{E}$ and ν are related to the dielectric constants and the effective masses respectively[1]. The E_λ^B is obtained from the relation[1-3]

$$E_\lambda^B = E_0 - E_\lambda \quad , \quad \lambda = 2_{p_0}, 3d_{\pm 1} \; , \tag{7}$$

where E_0 is the expectation value of H without tlie impurity terin. The hopping matrix is

$$V_{ij} =< \psi_i^\lambda(\vec{R}, z)|\phi(\vec{r})|\psi_j^\lambda(R, z) > \; . \tag{8}$$

Tlie density of states is given by

$$D(E) = -\frac{1}{\pi} Im \frac{1}{N} \sum_i G_{ii}(E + iO^+) > \; , \tag{9}$$

where $< G_{ii} >$ is the retarded single-particle propagator averaged on the impurities configuration[1,3,4]. \% calculated $D(E)$ through tlie relations

$$< G_{ii}(E + O^+) >= \xi(E)/E \; , \tag{10}$$

and

$$\eta(E) = \frac{N_{0x}\xi(E)}{(2\pi)^2 E^2} \int \frac{V^2(\vec{k}) d^2k}{1 - N_{0x}\xi(E)/EV(\vec{k})} \; . \tag{11}$$

Looking at Eq. (11), we see that we need $V(\vec{k})$, which is tlie Fourier transform of the hopping matrix V_{ij}. We can find, after some manipulation, that $V(\vec{k})$ can give all the information about tlie system to be considered. We obtain

$$V_\lambda(\vec{k}) = -(E_\lambda^B + q^2)\phi_\lambda^2(q) a^{*2} R_y^* \quad , \quad \vec{k} = \vec{q}/a^* \; . \tag{12}$$

Then:

$$V_{2p_0} = -\frac{(E_{2p_0}^B + a^{*2}k^2)\pi}{2a_0^2 \left(\frac{1}{4} + \frac{k^2 a^{*2}}{a_0^2}\right)^3} [a^{*2} R_y^*] \tag{13}$$

and

$$V_{3d_{\pm 1}}(k) = -(E_{3d_{\pm 1}}^B + a^{*2}k^2) \pi \left\{ \frac{1}{3a_1^2 F(\vec{k})^3} \left[\frac{9}{16F(\vec{k})^2} - \frac{6}{4F(\vec{k})} + 1 \right] \right\} \tag{14}$$

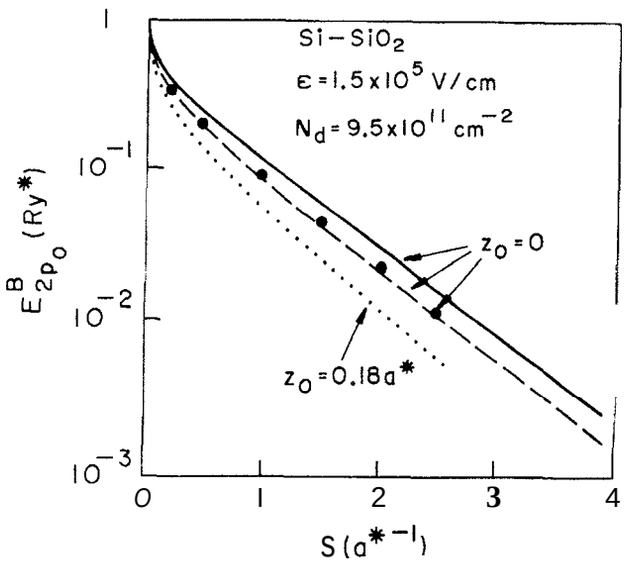

Figure 1. Binding energy of the $2p_0$, state as a function of tlie screening parameter. Full and dashed lines correspond to a: separable potential approximation and a modified Thomas-Fermi approximation respectively, calculated with the Klauder's multiple-scattering scheme[5]. The big and small dots are resiilts of our calculations.

where

$$F(\vec{k}) = \left(\frac{1}{4} + \frac{k^2 a^{*2}}{a_1^2}\right) \tag{15}$$

and $a^* = 21.8$ Å and $R_y^* = 42.3$ meV

II. Results

The binding energy for $2p_0$ state is shown in Fig.1, for specific electric field and depletion concentration N_d, and as a function of screening. The results are compared to recent results with Klauder's multiple-scattering approach[5]. In Fig. 2 we show the Fourier transform for $2p_0$ and $3d_{\pm 1}$ states for $s = 0$ and $z_0 = 0$.

At high electric field $\epsilon \geq 10^{10} esm = 3$ x 10^{12}V/cm, we find that, $E_{2p_0}^B \rightarrow 4R_y^*$ and $E_{3d_{\pm 1}}^B \rightarrow 4/9 R_y^*$. If we let $\vec{k} \rightarrow 0$ in Eqs. ***13*** and 14, $V_{2p_0}(\vec{k} = 0) \rightarrow V_{1s}(\vec{k} = 0)$, and and $V_{3d_+}(\vec{k} = 0) \rightarrow V_{2s}(\vec{k} = 0)$. Both systems go to the 1s and 2s states respectively, in the ideally two-dimensional systems, as obtained by Ghazali et al[6].

In Fig. 3 we show the density of states for $2p_0$ and $3d_{\pm 1}$ bands for different electric-fields and depletion concentrations, with $s = 0$ and $z_0 = 0$. The impurity concentration piesent in the $S, -S_iO_2$ inver ·on layer is

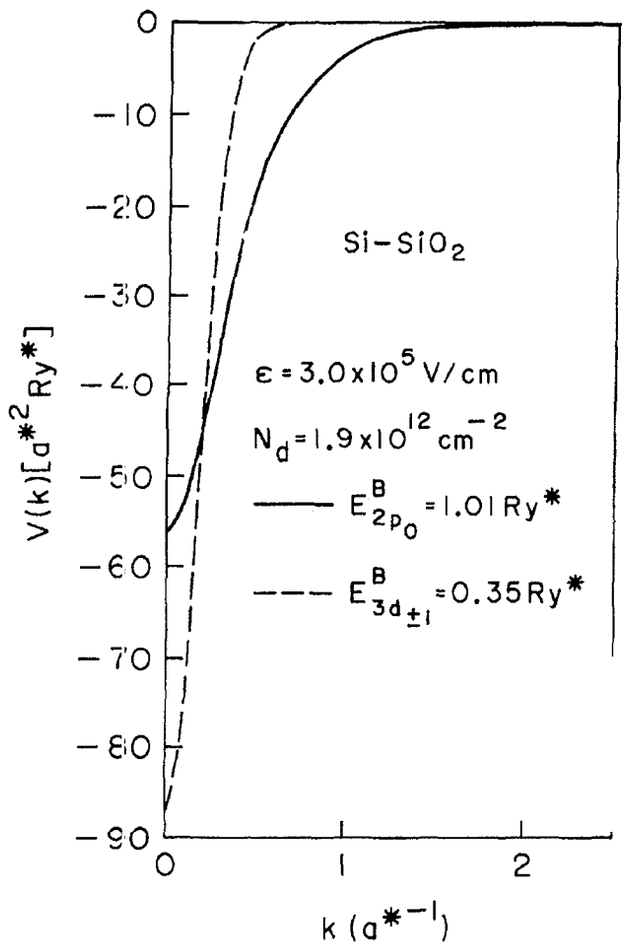

Figure 2. Fourier transform of tlie liopping eiiergy for the surface ground state $2p_0$ and tlie lowest excited state $3_{d_{\pm 1}}$.

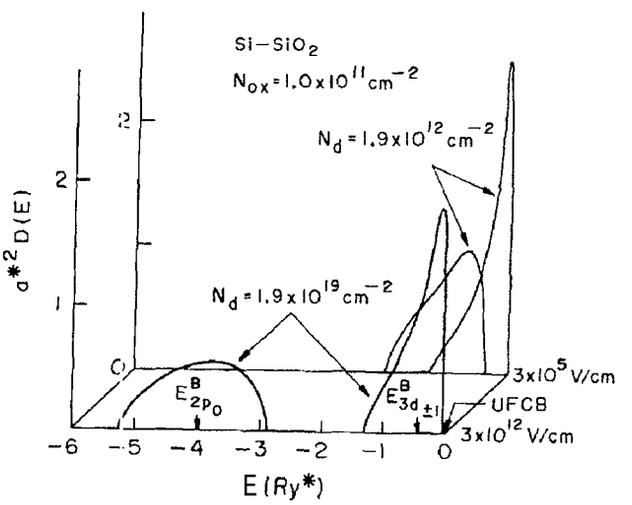

Figure 3. The calculated density of states for tlie $2p_0$ and $3d_{\pm 1}$ bands òr two differeiit electric-fields present in the $S,-S_iO_2$ iiiversion layer. The origin is sct at the unperturbed first conduc ion band (UFCB) and $s = 0$ and $z_0 = 0$.

$N_{ox} = 1 \times 10^{11}\text{cm}^{-1}$. The impurity bands for high electric field go to the ideally 2D separated bands[5,7]. The results can be compared to the 1s and 2s 2D states obtained by da Cunha Lima and Ferreira da Silva[7] and observed by Hartstein and Fowler[2,8]. The effects of correlation[9,10], screening and distance to the interface on tlie impurity bands are subject of current investigations and will appear elsewhere.

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