Two-dimensional impurity bands at semiconductor heterostructure interfaces

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A previously developed theory for electronic properties of doped semiconductors that uses a Hubbard-like Hamiltonian and takes into account the effect of disorder is applied to the impurity bands associated with inversion layers. It is shown that the impurity bands have a considerable bandwidth for concentrations in a range of experimental findings.

In this paper we consider the problem of impurity-band formation due to two-dimensional (2D) hydrogenlike bound states whose centers are randomly distributed on a plane surface.

We assume a Hubbard-like Hamiltonian

$$H = \sum_{i,j} V_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + \frac{U}{2} \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma} \ , \tag{1}$$

where $a_{i\sigma}^{\dagger}$ and $a_{i\sigma}$ refer to creation and annihilation operators of an electron with spin σ bound to an impurity assigned to the site i and $n_{i\sigma} = a_{i\sigma}^{\dagger} a_{i\sigma}$. V_{ii} is the ground-state energy (E_d) of the electron in the atomic limit, V_{ij} $(i \neq j)$ and U are, respectively, the hopping matrix associated with sites i and j and the intra-atomic correlation energy. They are given by

$$V_{ij} = -\int \psi(\vec{r} - \vec{R}_i) V(\vec{r} - \vec{R}_i) \psi(\vec{r} - \vec{R}_j) \, d^2 r \ , \tag{2}$$

and

$$U = \int |\psi(\vec{r}_i)|^2 \frac{e^2}{\bar{k}|\vec{r}_1 - \vec{r}_2|} |\psi(\vec{r}_2)|^2 d^2 r_1 d^2 r_2 \ , \tag{3}$$

where $\bar{k}$ is the dielectric constant and $V(r)$ is the contribution to the potential energy of the electron due to an impurity at site j.

We treat disorder according to the Matsubara-Toyozawa[1] (MT) theory for doped semiconductors. It seems to be a general property of tight-binding Hamiltonians for regular 2D lattices[2] that discontinuities appear in the density of states at the band edges together with divergences in the real part of the diagonal Green's function. As we will show later, the MT theory is very convenient to obtain information about those properties in the case of 2D structurally disordered tight-binding models.

It is well known that bound states due to sodium ions in the proximity of the Si-SiO$_2$ interface of a metal-oxide-semiconductor field-effect transistor (MOSFET) give rise to impurity bands at concentrations that vary between 10^{11}–10^{12} cm^{-2}.[3] Since the first calculation of these bound states by Stern and Howard[4] (SH) using the effective-mass theorem and considering a thickness inversion layer, many improvements have been achieved.[5]

Our present calculations of impurity bands correspond to the rather unrealistic case of the SH solution for the bound state with unscreened impurity potential and with the impurity located itself at the inversion layer. This rough treat-

ment generates 2D hydrogenlike bound states with binding energy equal to 4 Ry*. Although this oversimplification is unnecessary for the technique to be used it allows us to obtain analytic solution for the Fourier transform of the transfer matrix V_{ij}. We will leave improvements on the calculations of V_{ij} for a future paper. So, we take as ground state for the bound electron

$$\psi(r) = (8/\pi)^{1/2} a_0^{-1} \exp(-2r/a_0) \ , \tag{4}$$

where a_0 is the effective Bohr radius, $a_0 = \bar{k} h / m^* e^2$ and $\bar{k} = (\bar{k}_{ox} + \bar{k}_{Si})/2$. For the case of Si-SiO$_2$, 1 Ry$^* = 42$ meV.

Next, we apply a previously developed theory for impurity bands in doped semiconductors[6] based on a Mott-Hubbard model to the present 2D case. We define two Green's functions, $G_{ij\sigma}^+$ and $G_{ij\sigma}^-$ as

$$G_{ij\sigma}^{\pm}(t) = -i\Theta(t) \langle [a_{i\sigma} n_{i-\sigma}^{\pm}, a_{j\sigma}^{\dagger}(t)]_+ \rangle \ , \tag{5}$$

with $n_{i-\sigma}^+ = n_{i-\sigma}$ and $n_{i-\sigma}^- = 1 - n_{i-\sigma}$. The average Green's function results in

$$\langle G_{ii\sigma}^{\pm}(w) \rangle_{av} = \frac{n_{-\sigma}^{\pm}}{w - E^{\pm}} \xi^{\pm}(w - E^{\pm}) \ , \tag{6}$$

where $E^+ = E_d + U$, $E^- = E_d$ and

$$\xi^{\pm}(w) = 1 + \frac{\langle V_{ii} \rangle_{av}}{w - E^{\pm}} + \frac{\langle \sum_l V_{il} V_{li} \rangle_{av}}{(w - E^{\pm})^2} + \cdots \ . \tag{7}$$

In 2D, ξ obeys the equation

$$\xi^{\pm}(w) = \frac{1}{1 - \eta^{\pm}(w)} \ , \tag{8}$$

$$\eta^{\pm}(w) = \frac{N \xi^{\pm}(w)}{(2\pi)^2 w^2} \int \frac{V^2(\vec{k})}{[1 - N\xi^{\pm}(w)/w] V(\vec{k})} d^2 k \ . \tag{9}$$

In the above equation N is the number of impurities per cm^2 and $V(\vec{k})$ is the Fourier transform of the hopping potential:

$$V(\vec{k}) = \int \exp(i\vec{k}\cdot\vec{R}) V(\vec{R}) d^2 r \ . \tag{10}$$

Using Eq. (6), we have (from now on we will omit the symbol minus in G and ξ)

$$w \langle G_{ii\sigma}(w) \rangle = n_{-\sigma} \xi(w) \ . \tag{11}$$

Defining

$$\frac{\xi(w)}{w} = \frac{1}{Na_0^2(u+is)} \quad , \tag{12}$$

where a_0 is the effective Bohr radius, we have for the density of states $D(w)$

$$a_0^2 D(w) = \frac{1}{\pi}\frac{s}{u^2+s^2} \quad . \tag{13}$$

Now, bringing together Eqs. (8), (9), and (12), we have, after some manipulation

$$w = Na_0^2 u + \frac{2}{\pi}\int_0^\infty \frac{v^2(q)[u-v(q)]}{[u-v(q)]^2+s^2} q\,dq \quad , \tag{14}$$

and

$$Na_0^2 = \frac{2}{\pi}\int_0^\infty \frac{v^2(q)}{[u-v(q)]^2+s^2}\,dq \quad , \tag{15}$$

where $\vec{q} = \vec{k}/\alpha$ and $v(q) = a_0^2 V(\alpha q)$.

For regular 2D lattices, $\mathrm{Im}G_{ii}$ (a) shows discontinuities at $w = E_l$ and $w = E_u$, where E_l and E_u are the lower and upper band edges, respectively. On the other hand $\mathrm{Re}G_{ii}$ diverges at E_l and E_u.

In the above notation

$$\mathrm{Re}\langle G_{ii}(w)\rangle = \frac{1}{Na_0^2}\frac{u}{u^2+s^2} \quad , \tag{16}$$

and

$$\mathrm{Im}\langle G_{ii}(w)\rangle = -\frac{1}{Na_0^2}\frac{u}{u^2+s^2} \quad . \tag{17}$$

In order to fulfill the conditions on the real and imaginary parts of G_{ii}, we must have

$$s(w) = 0 \quad \text{for } E_l > w \text{ or } w > E_u \quad ,$$

$$u(w) \to 0 \quad \text{as } w \to E_l^- \text{ or } w \to E_u^+ \quad .$$

Bringing these results into Eq. (17) we see that the discontinuities lead to the unphysical result of $E_l = E_u = V(R=0)$. Therefore a finite bandwidth is not consistent with the discontinuity of the density of states at the band edge, at least in the formalism of Matsubara and Toyozawa.

After the pair of Eqs. (14) and (15) the Green's functions are obtained self-consistently. In case where an analytical expression for $V(\vec{k})$ is known, Eq. (9), instead can be used to provide an analytical solution for ξ.[7] Defining $\alpha = 2/a_0$ and $\vec{x} = \alpha\vec{R}$, and using Eqs. (2), (3), and (4), we get $V(x) = -8xK_1(x)$ Ry*, where $K_1(x)$ is the modified Bessel function of first order, and $U = 4.71$ Ry*. The Fourier transform of $V(\vec{R})$ is

$$V(k) = -\frac{128\pi a_0^2}{(4+a_0^2 k^2)^2}\ \mathrm{Ry}^* \quad . \tag{18}$$

Figure 1 shows the bandwidths of the lower and upper impurity bands, separated by U and their relative positions to the bottom of the inversion layer. Figure 2 shows the impurity bands for some concentrations, namely, $N = 1.55$, 3.10, and 6.20×10^{11} cm^{-2}.

It is evident that no discontinuity is observed on the band edges. However, a band tail pointing to the low-energy re-
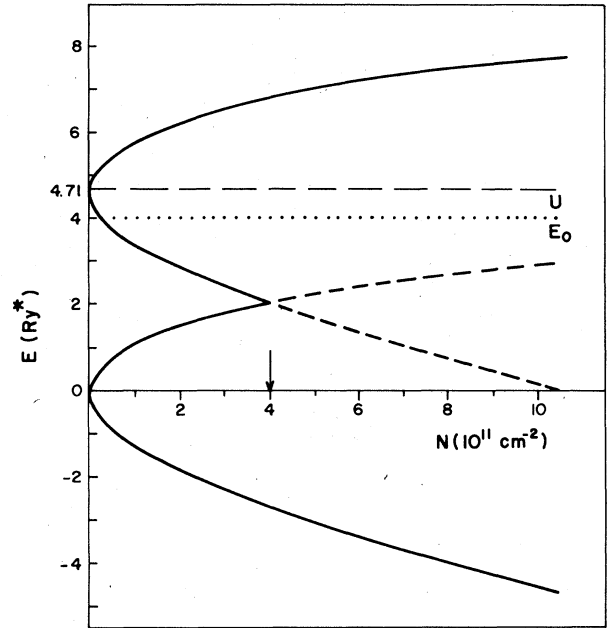

FIG. 1. Top and bottom edges of the 2D impurity bands as a function of the concentration N. The position of E_d is set at origin, as the location of the lower band. E_0 is the bottom of the inversion layer and U is the intra-atomic correlation energy. The arrow indicates the concentration at which the bands start overlapping.

gion characteristic of impurity bands in 3D is not observed in 2D bands. This feature does not seem to be a result of the approximation involved in the MT technique to treat disorder. It also appears when we use computer simulation of disorder and obtain the band by a cluster model.[8]

It is worthwhile to mention that Puri and Odagaki[9] calculated the one-band density of states using the homomorphic cluster coherent potential approximation. They have obtained no band tails for the 2D energy bands.

The overlapping of the two bands occurs at a concentration of 4×10^{11} cm^{-2}. At concentrations available for experiments[3], 1 to 3×10^{11} cm^{-2}, there is no overlapping but the bandwidth of the lower band is 50% to 100% of E_d.
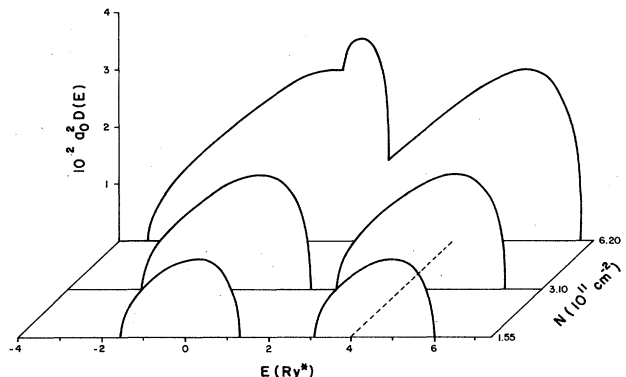

FIG. 2. Density of states of impurity bands as a function of concentration. E_d is set at the origin. Dotted lines refer to E_0.

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