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Density of impurity states associated with inversion layers

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In this paper we obtain the density of states for electrons bound to Na^+ impurities at the semiconductor-insulator interface of a metal-oxide-semiconductor structure, when an inversion layer is established by an external electric field. Impurity bands are calculated for several values of the screening length, the distance from the impurities to the inversion layer, and the impurity concentration. Results for the bandwidths and the peak values of the density of states are compared with experimental data.

I. INTRODUCTION

It seems to be well established by now that electrons in dynamically two-dimensional systems,[1] like metal-oxide-semiconductor (MOS) inversion layers, do not show a truly metallic conduction.[2] In these systems the conductivity shows a logarithmic divergence at very low temperature, even for extremely weak disorder, in what is generally called the weak-localization regime.[2,3] In a typical silicon MOS field-effect transistor (MOSFET) the roughness of the oxide-semiconductor interface is not important as a scattering mechanism when the applied gate voltage is not very high. In such cases disorder is mainly generated by impurity scattering, which is therefore the cause of localization. Impurities are also responsible for a tail in the conduction band, giving rise to activated conduction at low gate voltage.

Besides their importance in providing a scattering mechanism for conducting electrons, impurities in MOS structures have attracted attention because they allow the existence of bound states associated with the inversion layer. These bound states are much like shallow levels in doped semiconductors, and have been extensively studied both theoretically[1,4] and experimentally.[1,5]

It has been shown that sodium impurities (Na^+) can be made to drift through the oxide by an electric field and moved close to the oxide-semiconductor interface.[5] Samples have been produced for which the impurity concentration is fairly well known. When the concentration is increased the bound states at different sites start to overlap and a broadening of the energy level occurs. Such impurity-band formation below the first electron subband has, in fact, been observed in MOS structures.[6]

Impurity-band formation in heavily doped bulk semiconductors has been explored for the last two decades.[7] Much interest in this area is aimed at studying the metal-nonmetal transition.[8] It is commonly accepted that at high concentration two mobility edges occur inside the band, defining an interior range of extended states surrounded by regions where states are localized. When the concentration decreases, the two edges approach each other, an Anderson transition occurring when they coincide. A transition can also occur when the Fermi level crosses the mobility edge. However, at very high concentration, corresponding to a very large bandwidth, the Fermi level occurs at an energy for which a large number of extended states exist. It can happen that for such a situation the impurity potential is so strongly screened that no bound state is allowed to exist. In that case, impurities play the role of scattering centers for the conduction electrons and are also responsible for the conduction-band tailing.[9]

Impurity bands associated with inversion layers in a MOSFET should behave differently. Whenever the system is kept in the electrical quantum limit, i.e., as long as the electron system can be considered as dynamically two dimensional (2D), the impurity potential will always show at least one bound state, however large the screening. Therefore, the impurity band should always occur. In addition, because the density of states for the free carrier is independent of energy, the screening is independent of carrier concentration.

In this paper we study the impurity band associated with a 2D inversion layer, assuming the impurities are Na^+ charges randomly distributed close to the semiconductor-oxide interface. We start with bound states obtained according to the Stern-Howard (SH) theory.[4] The 2D system of electrons bound to an irregular lattice is described by a tight-binding model with structural disorder. The effect of disorder is worked out according to the Ishida-Yonezawa method.[10] This is shown in Sec. II. In Sec. III we show numerical results obtained for several distances from the Na^+ ion to the inversion layer and different screening parameters. In Sec. IV we present our comments on the results obtained and other considerations.

II. DENSITY OF STATES

The model for which our density of states is worked out consists of a set of impurities randomly distributed on a very thin sheet in the oxide at a distance z_0 from the inversion layer. We can consider, for instance, the impurities close to the oxide-semiconductor interface. We assume a very thin inversion layer, although this approximation could be relaxed in the theory after a few adjustments. We also assume that the electron-impurity interaction is screened by the free electrons according to the SH calculations. The attractive centers on the plane where the electrons are confined are given by the projection of the Na^+ ions on that plane and determined by position vectors $\mathbf{R}_l$. The one-electron Hamiltonian for a given impurity configuration is then

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + \sum_l V(\mathbf{r}-\mathbf{R}_l) \;, \tag{1}$$

where

$$V(\mathbf{r}) = -\frac{e^2}{\bar{\kappa}}(z_0^2+r^2)^{-1/2} + V_s(r) \;, \tag{2}$$

$$V_s(r) = \frac{e^2}{\bar{\kappa}} s \exp(sz_0) \int_d^\infty dz\,(z^2+r^2)^{-1/2}\exp(-sz) \;. \tag{2a}$$

In the above expression, $\bar{\kappa}=(\kappa_{\mathrm{ox}}+\kappa_{\mathrm{semic}})/2$, the average of the dielectric constants of the oxide and the semiconductor, and $V_s(\mathbf{r})$ is the potential term due to screening, given by (B18) of SH; $\mathbf{R}_l$ denotes the position of the projection of a particular impurity on the plane where the electrons are constrained to move.

To obtain the density of states, we attempt to calculate the Green's function for the above Hamiltonian in a tight-binding model, using as a basis the set of one-electron functions $\phi_l(\mathbf{r})=\phi(\mathbf{r}-\mathbf{R}_l)$, where $\phi(\mathbf{r})$ is the ground state of the single-site Schrödinger equation

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(r)\right]\phi(\mathbf{r}) = \epsilon\phi(\mathbf{r}) \;. \tag{3}$$

We solve numerically this equation for its ground state, for each value of z_0 and s, which are, respectively, the distance from the impurity to the inversion layer and the screening parameter. In particular, the solution of this equation for $z_0=0$ and no screening corresponds to the 2D hydrogen atom, with a binding energy of $4\mathscr{R}^*$ ($\mathscr{R}^*=42$ MeV for the $\mathrm{Si/SiO_2}$ interface).

The one-electron Green's function for the Hamiltonian (1) is defined by

$$(E-H)G(E) = 1 \;. \tag{4}$$

Here, $H=H_K+\sum_l V_l$, where H_K denotes the kinetic-energy operator and V_l the Coulomb and screening term corresponding to the impurity located at site $\mathbf{R}_l$.

Expanding $G(E)$ in terms of the functions $\phi_l(\mathbf{r}) = \langle \mathbf{r} \mid l\rangle$, we have

$$G(E) = \sum_{i,j} G_{ij}(E) \mid i\rangle\langle j \mid \;, \tag{5}$$

where the $G_{ij}(E)$ are unknown coefficients of the expansion. It is important to notice that this is essentially a one-band formalism. The extension of the results thus obtained to the multiband case is straightforward.[11] From (3)–(5), one obtains, after some manipulations, a set of coupled equations for the G_{ij}'s:

$$(E-\epsilon)G_{mj}(E) = \delta_{mj} + \sum_{\substack{l \\ (l\neq m)}} [T_{ml}-(E-\epsilon)S_{ml}]G_{lj}(E) \;, \tag{6}$$

where

$$T_{ml} = \langle m \mid V_m \mid l\rangle \tag{7}$$

and

$$S_{ml} = \langle m \mid l\rangle \;. \tag{8}$$

The basis we have used to describe our Hamiltonian is not orthogonal, i.e.,

$$S_{ml} = \int d^2r\,\phi(\mathbf{r}-\mathbf{R}_m)\phi(\mathbf{r}-\mathbf{R}_l) \neq \delta_{lm} \;.$$

In the derivation of (6) we have neglected, as usual, terms involving three-center integrals, i.e., terms like $\langle m \mid V_n \mid l\rangle$ with l,m,n all different. We have also neglected terms like $\langle m \mid V_i \mid m\rangle$ for $i\neq m$.[12]

Now, using a plane-wave expansion for the functions ϕ_l, we can express the trace of $G(E)$ as

$$\begin{aligned} \mathrm{tr}G(E) &= \sum_{\mathbf{k}} G_{\mathbf{kk}}(E) = \sum_{\mathbf{k}}\sum_{i,j} G_{ij}(E)\langle \mathbf{k} \mid i\rangle\langle \mathbf{k} \mid j\rangle^* \\ &= \sum_{\mathbf{k}} \left[\sum_i G_{ii}(E) \mid \langle \mathbf{k} \mid i\rangle \mid^2 \right. \\ &\qquad \left. + \sum_{\substack{i,j \\ (i\neq j)}} G_{ij}\langle \mathbf{k} \mid i\rangle\langle \mathbf{k} \mid j\rangle^* \right] . \end{aligned} \tag{9}$$

The impurity-band density of states is then given by

$$N(E) = -\frac{1}{\pi} I_m \lim_{\eta\to 0^+} \sum_{\mathbf{k}} G_{\mathbf{kk}}(E+i_\eta) \;. \tag{10}$$

What interests us is the average of $N(E)$ over all impurity configurations. We define the averaged trace of $G(E)$ as

$$\begin{aligned} \left\langle \sum_{\mathbf{k}} G_{\mathbf{kk}}(E) \right\rangle &= \sum_{\mathbf{k}} \left[\sum_i \int \frac{d^2R_i}{\Omega} \langle G_{ii}(E)\rangle_i \mid \langle \mathbf{k} \mid i\rangle \mid^2 \right. \\ &\qquad + \sum_{\substack{i,j \\ (i\neq j)}} \int \frac{d^2R_i}{\Omega} \int \frac{d^2R_j}{\Omega} \langle G_{ij}(E)\rangle_{ij} \\ &\qquad \left. \times \langle \mathbf{k} \mid i\rangle\langle \mathbf{k} \mid j\rangle^* \right] , \end{aligned} \tag{11}$$

where Ω is the area of the 2D system. The symbols $\langle \cdots \rangle_i$ and $\langle \cdots \rangle_{ij}$ denote conditional averages and are defined by

$$\langle G_{ii}(E)\rangle_i = \prod_{\substack{l \\ (l\neq i)}} \int \frac{d^2R_l}{\Omega} G_{ii}(E) \;, \tag{12}$$

$$\langle G_{ij}(E)\rangle_{ij} = \prod_{\substack{l \\ (l\neq i,j)}} \int \frac{d^2R_l}{\Omega} G_{ij}(E) \;. \tag{13}$$

For further comments about this approach in 3D systems, we refer the reader to the article by Yonezawa, Ishida, and Martino.[12] From now on we refer to the quantities (12) and (13) as the diagonal and off-diagonal averaged Green's functions, respectively. Because of the statistical homogeneity of the system, $\langle G_{ii}(E)\rangle_i$ is independent of i, and $\langle G_{ij}(E)\rangle_{ij}$ is a function of $\mathbf{R}_{ij}=\mathbf{R}_i-\mathbf{R}_j$ only:

$$\langle G_{ii}(E)\rangle_i=\overline{G}(E)\ , \tag{14}$$

$$\langle G_{ij}(E)\rangle_{ij}=\overline{G}(\mathbf{R}_{ij},E)\ . \tag{15}$$

Also, noting that

$$\langle \mathbf{k}\,|\,i\rangle=\int d^2r\frac{\exp(-i\mathbf{k}\cdot\mathbf{r})}{\sqrt{\Omega}}\phi_i(r)=\frac{\exp(i\mathbf{k}\cdot\mathbf{R}_i)}{\sqrt{\Omega}}\phi(\mathbf{k})\ , \tag{16}$$

we obtain, for the density of states per site,

$$\begin{aligned}D(E)&=\frac{N(E)}{N}\\&=-\frac{1}{\pi}\left[I_m\overline{G}(E)+\rho\int\frac{d^2k}{(2\pi)^2}\overline{G}(\mathbf{k},E)S(\mathbf{k})\right]\ ,\end{aligned} \tag{17}$$

where $\rho=N/\Omega$ is the impurity density and

$$S(\mathbf{k})=|\phi(\mathbf{k})|^2 \tag{18}$$

is the Fourier transform of the overlap integral

$$S(\mathbf{R})=\int d^2r\,\phi^*(\mathbf{r}-\mathbf{R})\phi(\mathbf{r})\ . \tag{19}$$

We obtain the diagonal and off-diagonal averaged Green's functions following the method developed by Matsubara and Toyozawa[13] (MT) for heavy doped semiconductors, which is briefly described in what follows.

Referring back to Eq. (6) and defining

$$V_{ml}(E)=[t_{ml}-(E-\epsilon)S_{ml}](1-\delta_{ml})\ ,$$

we can rewrite the equation of motion for G as

$$G_{ij}(E)=G^0_{ij}(E)+\sum_{k,l}G^0_{ik}(E)V_{kl}G_j(E)\ , \tag{20}$$

where

$$G^0_{ij}(E)=\delta_{ij}/(E-\epsilon)=\delta_{ij}G^0(E)$$

is the unperturbed Green's function, and V_{kl} is an effective perturbating hopping term. It can be shown that the diagonal matrix elements G_{ii} can be written in terms of a local self-energy as

$$G_{ii}(E)=[E-\epsilon-\Sigma_i(E)]^{-1}\ , \tag{21}$$

where

$$\begin{aligned}\Sigma_i(E)=&\sum_{l\,(\neq i)}V_{il}G^0(E)V_{li}\\&+\sum_{l\,(\neq i)}\sum_{m\,(\neq i)}V_{il}G^0(E)V_{lm}G^0(E)V_{mi}+\cdots\ .\end{aligned} \tag{22}$$

The summations that appear in each term are to be performed over all the impurities l, except the "home" impurity i.

Now, if in (22) we substitute the unperturbed Green's function associated with each intermediate site by the corresponding "dressed" one and restrict the summations in each term in a way that each impurity is visited only once in a given journey [this being denoted by the primes in Eq. (23) below], we obtain the series (23):

$$\begin{aligned}\Sigma_i^{\mathrm{MT}}(E)=&\sum_l{}'\,V_{il}G_{ll}(E)V_{li}\\&+\sum_l{}'\sum_m V_{il}G_{ll}(E)V_{lm}G_{mm}(E)V_{mi}+\cdots\ .\end{aligned} \tag{23}$$

On the other side, taking the configurational average of (21) and approximating $\Sigma_i(E)$ by $\Sigma_i^{\mathrm{MT}}(E)$, we obtain

$$\langle G_{ii}(E)\rangle\cong\langle[E-\epsilon-\Sigma_i^{\mathrm{MT}}(E)]^{-1}\rangle_i\ . \tag{24}$$

Now, replacing $\Sigma_i^{\mathrm{MT}}(E)$ by its configurational average, $\Sigma(E)$, and supposing that

$$\langle G_{mm}\rangle_{l,l_1,\ldots,l_\nu}=\overline{G}(E) \tag{25}$$

for any value of ν, we have

$$\overline{G}(E)=[E-\epsilon-\Sigma(E)]^{-1}\ , \tag{26}$$

where the averaged $\Sigma_i(E)$ is obtained by assuming that each site (impurity) position $\mathbf{R}_j$ runs over all of the plane with equal probability. Changing summations into integrals, we obtain

$$\begin{aligned}\Sigma(E)=\langle\Sigma_i^{\mathrm{MT}}(E)\rangle_i=&\frac{N}{\Omega}\overline{G}(E)\int d^2R_1\,V(\mathbf{R}_i-\mathbf{R}_1)V(\mathbf{R}_1-\mathbf{R}_i)\\&+\frac{N^2\overline{G}^{\,2}(E)}{\Omega^2}\int d^2R_1\,d^2R_2\,V(\mathbf{R}_i-\mathbf{R}_1)V(\mathbf{R}_1-\mathbf{R}_2)V(\mathbf{R}_2-\mathbf{R}_i)+\cdots\\=&\rho\overline{G}(E)\int\frac{d^2k}{(2\pi)^2}\frac{V^2(\mathbf{k})}{1-(N/\Omega)\overline{G}(E)V(\mathbf{k})}\ ,\end{aligned} \tag{27}$$

where

$$V(\mathbf{k})=\int d^2R\,\exp(i\mathbf{k}\cdot\mathbf{R})V(\mathbf{R})\ , \tag{28}$$

and from (26) and (27) we have a self-consistent equation for $\overline{G}(E)$:

$$\overline{G}(E)=(E-\epsilon)^{-2}+\rho(E-\epsilon)^{-1}G^{-2}(E)\int\frac{d^2k}{(2\pi)^2}\frac{V^2(\mathbf{k})}{1-\rho\overline{G}(\mathbf{E})V(\mathbf{k})}\ . \tag{29}$$

Furthermore, the off-diagonal Green's function can also be expressed in terms of $\overline{G}(E)$ following the same reasoning. Iterating expression (20) and applying the same path-eliminating procedure to it as we did to get (23), the series for $G_{ij}^{\mathrm{MT}}(E)$ is given by

$$G_{ij}^{\mathrm{MT}}(E)=G_{ii}(E)V_{ij}G_{jj}(E)+\sum_{l}{}' G_{ii}(E)V_{il}G_{ll}(E)V_{lj}G_{jj}(E)+\cdots \ . \tag{30}$$

Making use of (25), we can express the average of (30) as

$$\begin{aligned}\overline{G}(\overline{R}_{ij},E)=\langle G_{ij}^{\mathrm{MT}}(E)\rangle_{ij}=\overline{G}^{\,2}(E)V(\mathbf{R}_{ij})+\overline{G}^{\,3}(E)\rho\int d^2R_1\, V(\mathbf{R}_i-\mathbf{R}_1)V(\mathbf{R}_1-\mathbf{R}_j)&\\ +\overline{G}^{\,4}(E)\rho^2\int d^2R_1\, d^2R_2\, V(\mathbf{R}_i-\mathbf{R}_2)V(\mathbf{R}_1-\mathbf{R}_2)V(\mathbf{R}_2-\mathbf{R}_j)+\cdots \ ,&\end{aligned} \tag{31}$$

and its Fourier transform as

$$\overline{G}(\mathbf{k},E)=\overline{G}^{\,2}(E)V(\mathbf{k})/[1-\rho\overline{G}(E)V(\mathbf{k})] \ . \tag{32}$$

Equations (29) and (32) are self-consistent equations that must be solved numerically to obtain $\overline{G}(E),\overline{G}(\mathbf{k},E)$ for each value of E. The density of states is then obtained from (17).

Our only remaining task is to obtain $V(\mathbf{k})$ for our particular system. The hopping integral $T_{ml}=\langle m \mid V_m \mid l\rangle$ is given by

$$T_{ml}=T(\mathbf{R}_m-\mathbf{R}_l)=\int d^2r\, \phi^*(\mathbf{r})V(\mathbf{r})\phi(\mathbf{r}-\mathbf{R}_{ml}) \ . \tag{33}$$

Using the Schrödinger equation (3) and Fourier transforming, we obtain

$$\begin{aligned}T(\mathbf{k})&=\int d^2R \exp(-i\mathbf{k}\cdot\mathbf{R})\\ &\quad\times\int d^2r\, \phi^*(\mathbf{r})\left[\epsilon+\frac{\hbar^2}{2m^*}\nabla^2\right]\phi(\mathbf{r}-\mathbf{R})\\ &=\left[\epsilon-\frac{\hbar^2k^2}{2m^*}\right]\phi^2(\mathbf{k}) \ ,\end{aligned} \tag{34}$$

and therefore

$$\begin{aligned}V(\mathbf{k})&=[T(\mathbf{k})-(E-\epsilon)S(\mathbf{k})]\\ &=\left[2\epsilon-E-\frac{\hbar^2k^2}{2m^*}\right]\phi^2(\mathbf{k}) \ .\end{aligned} \tag{35}$$

It is worth mentioning that the effect of screening by free carriers has been considered throughout all the calculations and not only in the determination of the single-impurity eigenstates. This can be seen directly from the calculation of the hopping integral, Eqs. (33) and (34), where screening is taken into account not only in the wave function $\phi(\mathbf{r})$, but also in the potential $V(\mathbf{r})$ given by Eq. (2).

III. RESULTS

Following the procedure outlined in Sec. II, we performed numerically the following steps for each pair z_0,s (the distance from the impurities to the inversion layer and the inverse screening length, respectively): (1) Evaluate the screened Coulomb potential of one impurity, $V(r)=V_c(r)+V_s(r)$; (2) solve the Schrödinger equation (3) to obtain ϵ and $\phi(r)$ for the ground state; (3) Fourier-transform $\phi(r)$ to obtain $\phi(k)$, $T(k)$, and $S(k)$; (4) using the effective hopping term $V(k)$ in Eq. (35), solve the integral equation (29) for $\overline{G}(E)$, thus obtaining $\overline{G}(\mathbf{k},E)$ from Eq. (32); and (5) obtain the density of states for the impurity band using Eq. (17).

The radial Schrödinger equation for the radially symmetric $\phi(r)$ was solved using the method by Noumerov.[14] The Fourier transform $\phi(k)$ was obtained according to

$$\phi(k)=\int_{-\infty}^{+\infty}\exp(ikx)P(x)dx \ , \tag{36}$$

with

$$P(x)=\int_{-\infty}^{+\infty}dy\, \phi(x,y) \ , \tag{37}$$

where we have used the fact that $\phi(\mathbf{k})$ is radially symmetric. Equation (36) was solved numerically using a fast-Fourier-transform (FFT) subroutine. The density of states so obtained was always found to be correctly normalized with an accuracy of at least 99%.

The total impurity potential $V(r)$ and the screening contribution $V_s(r)$ are shown in Fig. 1. It can be seen that for each value of z_0 the potential well gets simultaneously

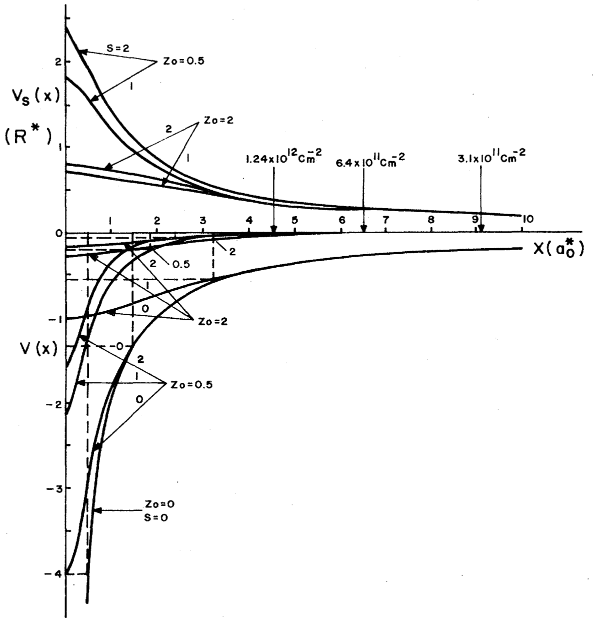

FIG. 1. Impurity Coulomb potential $V(x)$ for the interface Si/SiO$_2$, for various values of z_0 and s. $V_s(x)$ is the screened Coulomb potential. The arrows indicate the mean separation of impurities for different ρ. The dashed lines correspond to the ground-state energies and their corresponding classical radii for z_0 and s, respectively.

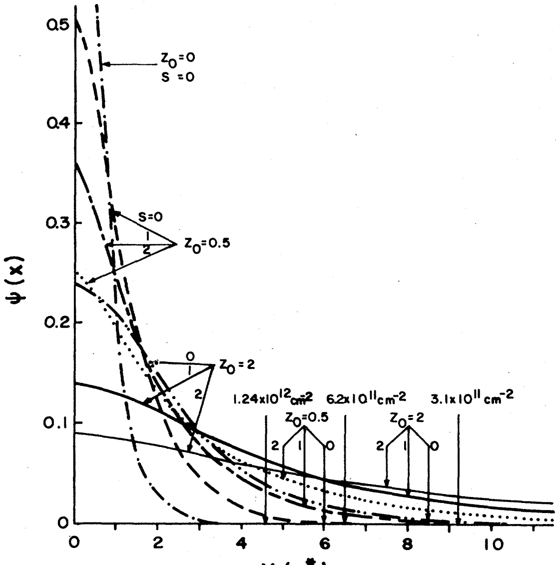

FIG. 2. Wave functions for the semiconductor-insulator interface, when the impurity is located at a distance z_0 from the inversion layer surface and has a screening constant s. The arrows indicate the mean separation of impurities for different concentrations ρ. The effective Bohr radius used was $a_0^*=22$ Å.

narrower and shallower as the screening length decreases (i.e., s increases). The behavior of $V(r)$ is reflected in the behavior of the ground-state wave function $\phi(r)$, shown in Fig. 2. For each value of z_0 (s), the wave function gets broader for increasing s (z_0).

The behavior of the impurity density of states is analyzed next. Figure 3 shows the calculated density of states for an unscreened impurity potential ($s=0$) and 1.55×10^{11} impurities per cm^2 for several values of z_0. A typical feature of these bands is their asymmetry, with tails pointing to the higher-energy side. The asymmetry increases with increasing z_0, and at $z_0=2$ the impurity band overlaps considerably with the conduction band (first electron subband). However, we should call attention to the fact that we have neglected the so-called ionic terms in the diagonal matrix elements of the Hamiltonian, terms like $\langle m \mid V_i \mid m \rangle$, for $i \neq m$. Those terms, if not cancelled out by the contribution of the negative-charge interaction, should shift the peak of the impurity band. In a first attempt SH have estimated the concentration at which the impurity band would merge in the conduction band. They found $\rho=9\times10^{11}$ cm^{-2} for $d=2$ and $s=0$ in Si, a value that is much bigger than what is expected if our approximations are reasonable.

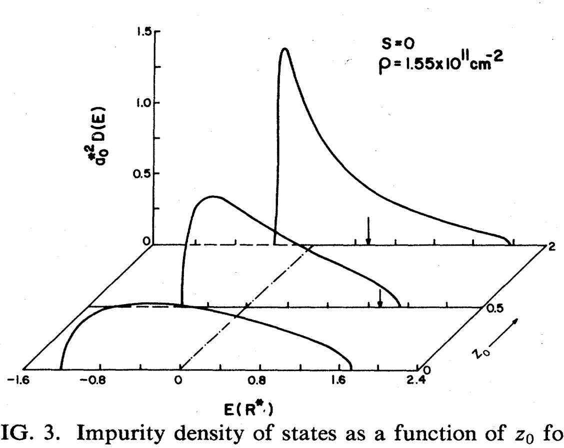

FIG. 3. Impurity density of states as a function of z_0 for an unscreened impurity potential ($s=0$) and $\rho=1.55\times10^{11}$ cm^{-2}. The arrows indicate the bottom of the conduction band (first electron subband) E_0.

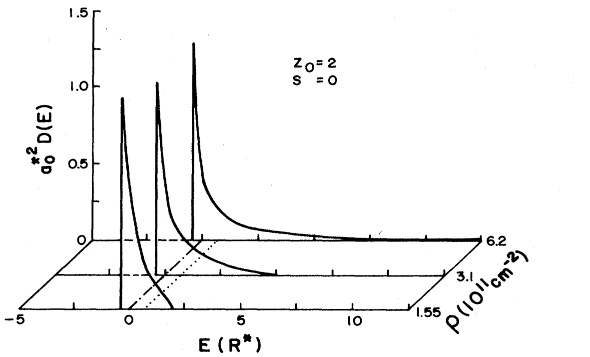

FIG. 4. Impurity density of states as a function of concentration for $z_0=2$ and $s=0$. Dotted lines refer to $E_0=0.5406$.

The effect of changing the impurity concentration is exemplified in Figs. 4 and 5. In Fig. 4, which the screening neglected, the expected behavior is observed, namely the band gets broader with increasing impurity concentration. This effect persists when screening is taken into account, as seen in Fig. 5. However, the screening in the SH theory is considered to be caused by electrons in the conduction band. The screening length is then a constant proportional to the density of states at the Fermi energy of a 2D electron gas. This model should apply only for the case in which the Fermi level is deep inside the conduction band, i.e., when N_s, the electron concentration of the 2D system, is far bigger than ρ, the impurity concentration. This is certainly not the case for the experimental studies[1] that obtain the impurity-band density of states from activated mobility measurements and N_s is of the order of ρ.

Because of the considerations above and due to the lack of a good theory for screening by localized states, the inverse screening length has been treated as a free parameter. Figure 6 shows impurity bands calculated for a fixed concentration of impurities and z_0 for several values of s. The values appropriate for the [100] surfaces of InAs, Si, and Ge are $s=2$, 4, and 8, and $z_0=0.25$, 2, and 1, respec-

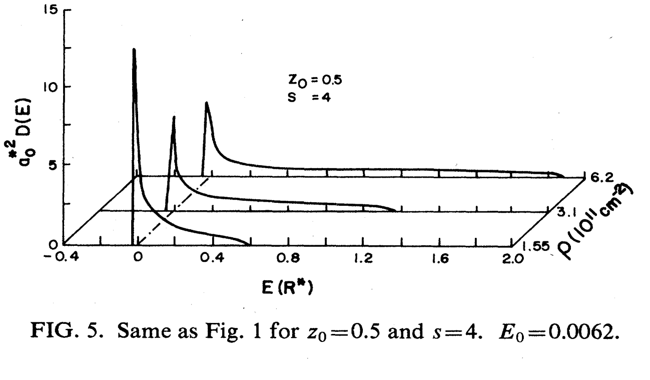

FIG. 5. Same as Fig. 1 for $z_0=0.5$ and $s=4$. $E_0=0.0062$.

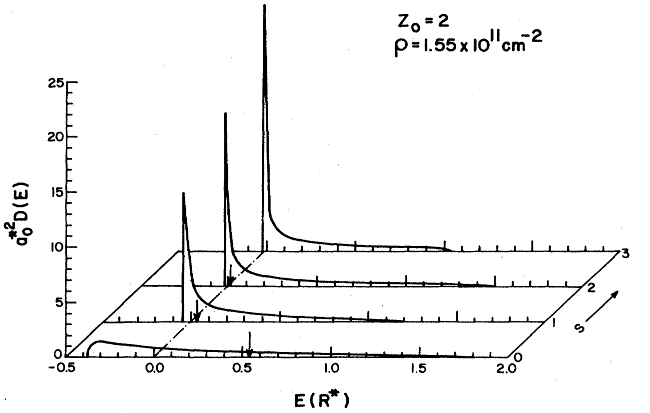

FIG. 6. Impurity density of states as a function of s for $\rho = 1.55 \times 10^{11}$ cm^{-2} and $z_0 = 2$. The arrows indicate the bottom of the first electron subband.

tively, assuming that the impurities lie on the interface. It is seen from Fig. 6 that the density of states is very sensitive to the value of s.

To summarize the behavior of the density of states with z_0, we have plotted in Fig. 7 the dispersion of the impurity band as a function of z_0 for several typical values of the impurity concentration. The dispersion is a measure of the bandwidth and is defined by the cumulant

$$\Gamma = \left[\int dE (E^2 - \bar{E}^2) N(E) \Big/ \int dE \, N(E) \right]^{1/2} .$$

For very low impurity concentration, in which case the overlap can be neglected, the behavior of the density of states can be inferred from the behavior of the hopping term $T(R)$. However, in the experimentally feasible range of impurity concentrations, such is not the case. Equations (29) and (32) show how complicated the dependence of the bandwidth on the parameters z_0 and s is. As a consequence, the bandwidth does not show a monotonic dependence on either z_0 or s, as can be seen from Figs. 6 and 7.

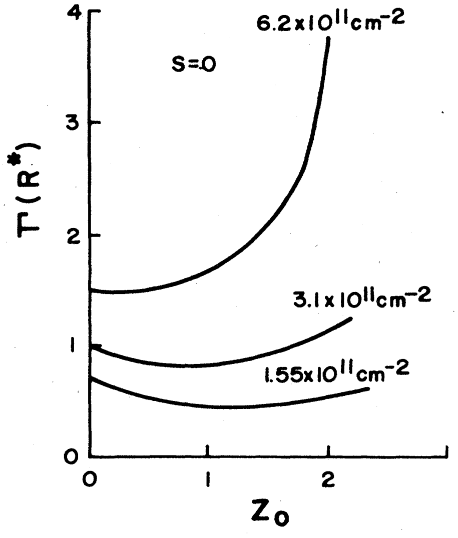

FIG. 7. Variation of the impurity-density-of-states dispersion with the concentration and z_0 for $s = 0$.

Despite the oversimplifications inherent in the model we used, we can compare our results with some values obtained experimentally. The peak value of the density of states for the Si/SiO$_2$ MOSFET, with $\rho = 3.5 \times 10^{11}$ cm^{-2}, is quoted by Ando *et al.*[1] to be 3.4×10^{18} cm^{-2} eV^{-1}, associated with a bandwidth of 1.8 meV. We have found these same parameters to be $D(E)_{\max} = 1.62 \times 10^{14}$ cm^{-1} eV^{-1} and $\Gamma = 44$ MeV for $z_0 = 2$ and $s = 0$, with $\rho = 3.1 \times 10^{11}$ cm^{-2}. In a more recent work, Hartstein and Fowler[15] found the density of states to be an order of magnitude broader than inferred from their earlier measurements. This brings their results much closer to the values we have obtained. They have obtained the value for $D(E)_{\max}$ by fitting the density of states to a Gaussian distribution with half-width Γ. We have seen that the curve we obtained is highly asymmetric with a long tail at the higher-energy side. This makes a Gaussian a very bad choice, resulting in a very small value for the peak.

We should comment on the asymmetry a bit more. It can be seen from Figs. 4 and 5 that the band tail is very big and the distribution very sharp for large z_0 and s. This asymmetry is typical of the structural disorder and the tail on the right-hand side is a consequence of the bases we took to represent our impurity system. However, since the impurity-band tail overlaps the conduction band, the hybridization between them pushes the impurity band down and creates resonant states inside the first electron subband.[16] This effect has been considered already in 3D systems like heavily doped semiconductors.[9,17]

IV. CONCLUSIONS

We have calculated the impurity-band density of states (DOS) for Na$^+$ impurities located near the oxide-semiconductor interface of an MOS structure. We have assumed the one-impurity ground state as given by SH theory. This work is the first attempt at exploring the one-electron tight-binding formalism in the description of impurity states associated with inversion layers. The main shortcomings of this treatment are the Thomas-Fermi approximation for the electron-ion potential and the assumption of cancellation between the ionic terms and the Coulomb term of the electron-electron interaction. These result in a poor prediction for the position of the center of gravity of the impurity band. Nevertheless, we think that the main features of the results, namely the bandwidth and the peak value of the DOS, are not very sensitive to these approximations.

Finally, the system described here is an impurity band in the presence of a partially occupied conduction band (first electron subband). This is not the same as what is usually investigated in experiments.[1] There, the impurity DOS is inferred from activated conductivity measurements as the Fermi level is swept through the impurity band. An experiment more closely related to this model would be an optical-absorption experiment involving transitions from the occupied impurity states to unoccupied states far above them, in the conduction band.

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