Impurity density of states in n-type Si inversion layers

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(Received 1 September 1992)

We calculate the impurity density of states for electrons bound to impurity centers localized inside the oxide and at the interface of the metal-oxide-semiconductor system. The screening and the disorder effects are taken into account in the calculation. We show that for a given impurity concentration, electric field, and binding energy of experimental interest, the ground-state band remains separated from the unperturbed band and starts to overlap the lowest excited band.

Recently there has been considerable interest in the investigation of impurities in inversion layers of metal-oxide-semiconductor (MOS) structures. Impurity bands have been found experimentally in these structures. It is well known that such bands have important consequences in optical and transport measurements.[1,2]

The main purpose of the present work is to show how in an n-type Si inversion layer the ground-state band, the lowest excited band, and the unperturbed first conduction subband edge, subject to disorder, screening, and electric field, evolve as the impurity concentration is increased, up to a concentration of experimental interest.[3-7]

We assume the Hamiltonian in a random, one-body tight-binding approximation, with monovalent impurities as

$$H=E_{\lambda}^{B}\sum_{i}|i\rangle\langle i|+\sum_{i\neq j}V_{ij}|i\rangle\langle j| \ , \tag{1}$$

where E_{λ}^{B} is the binding energy, which is taken as our reference energy below the edge of the first conduction subband, λ are the states to be considered, and V_{ij} is the random energy integral.

The density of states (DOS) are calculated from the Green's functions[4]

$$G_{ij}^{(\pm)}(\omega)=\langle 0|a_i\frac{1}{\omega-H\pm i\delta}a_j|0\rangle \ , \tag{2}$$

with the configuration averaging over a random distribution of impurities. We treat this configurational average according to the Matsubara-Toyozawa scheme for doped semiconductors.[8]

It is easy to show that we may reach the coupled equations, in our two-dimensional version, as[4,8]

$$\xi=(1-\eta)^{-1} \ ,$$
$$\eta=1-\frac{1}{\xi(\omega)}=\frac{N_{\rm ox}\xi(\omega)}{4\pi^2\omega^2}\int\frac{V^2(\mathbf{k})d^2k}{1-N_{\rm ox}\xi(\omega)/\omega V(\mathbf{k})} \ , \tag{3}$$

where $N_{\rm ox}$ is the inversion layer impurity concentration per square centimeter and $V(\mathbf{k})$ is the Fourier transform of V_{ij}.

For the Si-SiO_2 system we adapt the units $R_y^*=42.3$ meV and $a^*=21.8$ Å. We get the binding energy from variational solution for the isolated impurity as[3]

$$E=\langle\psi|-\nabla_{x,y}^2-\nu\nabla_z^2+\frac{\delta}{z}+\epsilon z-2\Phi(\mathbf{r})|\psi\rangle \ , \tag{4}$$

where ϵ is the external electric field, $\Phi(\mathbf{r})$ is the screened Coulomb potential, and δ and ν are related to the dielectric constants and the effective masses, respectively. Then we get E_{λ}^{B} from the relation[3]

$$E_{\lambda}^{B}=E_0-E_{\lambda}, \quad \lambda=2p_0,\ 3d_{\pm1} \ , \tag{5}$$

where E_0 is the energy value without impurity. The wave function is given by[3]

$$\psi(\mathbf{r},z)=(a^2/2\pi)^{1/2}\exp(-ar/2)(b^3/2)^{1/2}z\exp(-bz/2) \ , \tag{6}$$

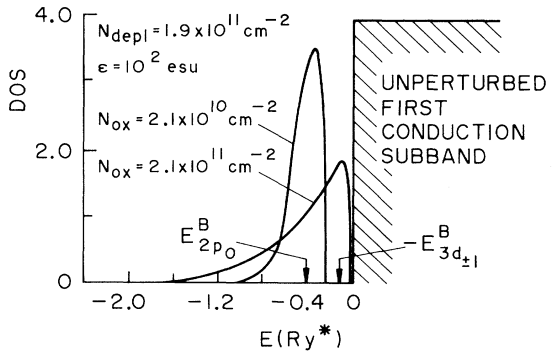

FIG. 1. The calculated density of states for the $2p_0$ band for two different concentrations of impurities $N_{\rm ox}=2.1\times10^{10}$ cm^{-2} and $N_{\rm ox}=2.1\times10^{11}$ cm^{-2} present in the Si-SiO_2 inversion layer. The arrows indicate the binding energies of the $2p_0$ and $3d_{\pm1}$ states, respectively.

and the hopping term V_{ij},

$$V_{ij}=\int dz \int d^2r\, \psi_i(r,z)V_i(\mathbf{r},z)\psi_j(r,z)\ , \tag{7}$$

where V_i is the Coulomb potential.

The results for the $2p_0$ DOS are shown in Fig. 1, for two different impurity concentrations. The values used in the calculation are screening $s=0.04$, distance of the impurity to the interface $z=0.14$, $E^B_{2p_0}=0.4R^*_y$, $E^B_{3d_{\pm 1}}=0.12$, and $\epsilon=10^2$ esu. The depletion layer concentration for this ϵ is found to be $N_{\rm depl}\simeq 2\times 10^{11}$ cm^{-2}.

We observe that for $N_{\rm ox}\simeq 2\times 10^{10}$ cm^{-2} the $2p_0$ DOS is quite symmetrical and separated from the unperturbed first conduction subband edge (UFCS) and it would start to overlap the $3d_{\pm 1}$ band. As the concentration increases the DOS gets more asymmetric and close to the edge of the UFCS, crossing it at a 2×10^{11} cm^{-2}. Such effects have, in fact, been observed experimentally.[2-5]

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