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14. Abstract/Notes

We calculate the density of states (DOS) for N_a^+ impurity bands in n-type Si/SiO_2 MOS structures with a Hubbard-like model and using as a basis Martin and Wallis single-impurity states. We show that the intrasite correlation energy increases with the applied electric field on the junction. The same occurs with the bandwidth and with the energy corresponding to the maximum in the DOS. This effect is enhanced by increasing the impurity concentration, N_{ox}. The asymmetry of the DOS explains why the measured binding energy for finite N_{ox} is smaller than in the single-impurity case.

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RESUMO

Calcula-se a densidade de estados da banda de impureza de N_a^+ em MOS do tipo n através do modelo de Hubbard, usando como base a solução de Martin e Wallis para o problema de uma impureza. Mostra-se que a energia de correlação intra-sítio cresce com o campo aplicado na interface Si/SiO_2. O mesmo ocorre com a largura da banda e com a energia do máximo da densidade de estados. Este efeito vai ficando mais pronunciado com o aumento da concentração de impurezas N_{ox}. A assimetria na curva da densidade de estados explica porque a energia de ativação medida é menor que a energia de ligação.

Impurity bands in n-type Si/SiO_2 MOS

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Abstract

We calculate the density of states (DOS) for Na^+ impurity bands in n-type Si/SiO_2 MOS structures with a Hubbard-like model and using as a basis Martin and Wallis single-impurity states. We show that the intrasite correlation energy increases with the applied electric field on the junction. The same occurs with the bandwidth and with the energy corresponding to the maximum in the DOS. This effect is enhanced by increasing the impurity concentration, N_{ox}. The asymmetry of the DOS explains why the measured binding energy for finite N_{ox} is smaller than in the single-impurity case.

It is well-known that electrons in inversion layers (IL) of metal-oxide-semiconductor (MOS) structures are a good way to study transport properties of disordered systems such as metal nonmetal transtion, weak localization, quantum Hall effect etc.[1] Another relevant question concerns the existence of an impurity band in those structures, associated with an activated transport regime at low temperatures. In fact, the occurrence of impurity band in n-type Si/SiO_2 MOS has been observed by Hartstein and Fowler (H-F)[2] and more recently by Glaser et al.[3] The band is usually generated by the presence of Na^+ ions that are randomly located near the interface in the oxide region and which bind electrons in the semiconductor.

The electronic states associated with Na^+ impurities in Si/SiO_2 MOS have been studied theoretically in the past by several authors[4-7]. Among other factors, the states depend on the electric field that is applied perpendicular to the junction in order to form the depletion layer. Unlike impurity bands in doped semiconductors, the position of the Fermi level, which in that case depends only on the impurity concentration, in the case of MOS it is determined by the gate voltage and by the substrate bias. Therefore the Fermi level can be made to scan the impurity band allowing, in consequence, an external control of the filling factor, i.e., the average number of electrons per impurity. Another interesting feature from a theoretical point of view is the possibility of varying the electronic intrasite (impurity) interaction potential with the gate voltage. In a Hubbard-like model Hamiltonian representing the impurity electrons, it would correspond to control externally the correlation U and its ratio to the bandwidth Δ.

In a first attempt to calculate the density of impurity states (DOS) associated with an IL, da Cunha Lima et al.[6] used a tight binding model based on a single-impurity state given by the two-dimensional effective mass approximation of Stern and Howard[4]. However, more realistic treatments exist for the one-impurity problem[5-7], which take into account important corrections such as: an image charge potential due to a large difference between the dielectric constants of the oxide and semiconductor; the spatial extension in the z-direction (normal to the interface) of the electron wave function; and the dependence of the bound state on external applied field. In the present calculation we used the variational solution due to Martin and Wallis (M-W)[5]. It does not consider screening of the impurity potential due to IL electrons. However, for the purpose of calculating the impurity band, this is a reasonable assumption, since the latter is determined generally by measuring the activated conductivity and in this case the Fermi level lies below the first subband. On the other hand, a variational solution for the single-impurity problem makes the DOS calculation much easier. A more accurate treatment should consider the screening due to a finite density of states at the Fermi level. Nevertheless, these states would correspond to electrons in the impurity band, certainly localized, which screen the impurity potential very weakly.

In the model considered here we include electron-electron correlation via a Hubbard-like Hamiltonian:

$$H = \sum_{i\sigma} \varepsilon\, a^{+}_{i\sigma} a_{i\sigma} + \sum_{i\neq j} V_{ij} a^{+}_{i\sigma} a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \quad , \qquad (1)$$

where $a^+_{i\sigma}$ and $a_{i\sigma}$ refer to creation (anihilation) operators of an electron with spin σ in the bound state described by a M-W wave function, ψ_i, centered at the impurity i:

$$\psi_i(\vec{r},z) = \phi_i(\vec{r})\xi(z) = (a^2/2\pi)^{1/2}\, e^{-ar/2}(b^3/2)^{1/2}\, ze^{-bz/2} \quad . \tag{2}$$

The single impurity Hamiltonian depends on the electric field through the carrier concentration of the depletion layer N_{depl}. The dependence of the DOS on the electric field comes out through the variational parameters a and b. V_{ij} is the hopping matrix element,

$$V_{ij} \equiv \int dz \int d^2r\ \psi_i(\vec{r},z) v_i(\vec{r},z) \psi_j(\vec{r},z) \quad , \tag{3}$$

where v_i is the interaction potential between the electron and an impurity located at site $\vec{R}_i$. We assume that the impurities lie at z = 0.

The DOS is now obtained calculating the single-particle Green's function via a method previously developed by Kishore[9] and applied to doped semiconductors by Ferreira da Silva et al[10]. The configurational average uses the diagrammatic summation of Matsubara and Toyozawa (M-T)[11]. Defining

$$G^{\pm}_{ij,\sigma}(t) = i\theta(t) < [a_{i\sigma} n^{\pm}_{i-\sigma}, a^+_{j\sigma}(t)]_+ > \tag{4}$$

with $n^+_{i\sigma} \equiv a^+_{i\sigma} a_{i\sigma}$ and $n^-_{i\sigma} = 1 - n^+_{i\sigma}$, we have for the single-particle GF the sum of G^+ and G^-. The lowest order approximation in the Kishore's method[9] gives an equation of motion for $G^{\pm}$ in first order of U:

$$(\omega - E^{+})G^{\pm}_{ij,\sigma}(\omega) = n^{\pm}_{-\sigma}\delta_{ij} + \sum_{\ell\neq i} V_{i\ell}G^{\pm}_{\ell j\sigma}(\omega) \quad , \tag{5}$$

where $E^{+} = \varepsilon + U$, $E^{-} = \varepsilon$, and we have assumed $n^{\pm}$ as site independent. The configuration averaged diagonal elements for impurities in a plane are[12]:

$$\langle G^{\pm}_{ii,\sigma}(\omega)\rangle_{av} = \frac{n^{\pm}_{-\sigma}}{\omega - E^{\pm}} \; \xi^{\pm}(\omega) \quad , \tag{6}$$

$$\xi^{\pm} = [1 - \eta^{\pm}(\omega)]^{-1} \quad , \tag{7}$$

$$\eta^{\pm}(\omega) = \frac{N_{ox}\; \xi^{\pm}(\omega)}{(2\omega)^2(\omega-E^{\pm})^2} \int d^2k \; \frac{V^2(\vec{k})}{1 - [N\xi^{\pm}(\omega)/(\omega-E^{\pm})]\; V(\vec{k})} \quad , \tag{8}$$

where N_{ox} is the number of impurities per cm² and $V(\vec{k})$ is the 2-D Fourier transform of the hopping potential $V(\vec{R})$ in Eq. (3). The pair of Eqs. (7, 8) is now solved numerically to obtain the density of states for the upper and lower Hubbard bands, D^{+} and D^{-}:

$$D^{\pm}(\omega) = -\frac{N}{\pi}\sum_{\sigma}\mathrm{Im}\langle G^{\pm}_{ii,\sigma}(\omega + i0^{+})\rangle_{av} \quad . \tag{9}$$

The problem is then reduced to the calculation of U and $V(\vec{k})$.

Using the usual atomic units appropriate for the (100) n-type Si/SiO_2 IL, $Ry^* = 43.6$meV and $a^*_0 = 21.7$Å, we obtain:

$$V(\vec{k} = \vec{q}/a^*) = -(E_b + q^2)\phi^2(q)a^{*2}_0 \; Ry^* \quad , \tag{10}$$

where E_b is the binding energy for the single-impurity and $\phi(q)$ is given by

$$\phi(q) = \int e^{-i\vec{q}\cdot\vec{x}}\phi(r = xa_0^*)d^2x \quad . \tag{11}$$

After performing the integral above, we get:

$$V(k) = -(E_b + a^{*2}k^2)\pi \left[2a^2 \left(\frac{1}{4} + \frac{a_0^{*2}k^2}{a^2} \right)^3 \right]^{-1} a_0^{*2}Ry^* \quad . \tag{12}$$

The intrasite correlation energy $\langle ii|V(\vec{r}_1 - \vec{r}_2)|ii\rangle$ is calculated numerically using a potential $V(\vec{r}_1 - \vec{r}_2)$ that takes into account the image charge due to the difference in the dielectric constants of the semiconductor and the oxide[13]. As a result we obtain a correlation energy U depending on the applied electric field, as shown in Fig. 1. In the range realizable in the experiments, U is greater than E_b, what explains why the upper Hubbard band is not observed, as already pointed out by da Cunha Lima and Ferreira da Silva[12]. It is worthwhile to say that U does not go to the 2-D limit of 4.17 Ry* for very high field. This is due to the addition of the image term in the interaction potential.

The calculated DOS is shown in Fig. 2. We have chosen $N_{depl} = 0.36 \times 10^{12}cm^{-2}$ in order to compare with the results obtained by H-F. The zero in energy corresponds to the single-impurity ground state. We have also assigned the position of the IL first subband. The peak of the lower band is dislocated to the right of the zero of energy, what explains why the measured binding energy for finite N_{ox} is smaller than for the single-impurity. We can also observe that, for $N_{ox} = 5.0 \times 10^{11}cm^{-2}$ the lower band has already merged into the conduction band. H-F found, by extrapolation, $E_b = 0$ for $N_{ox} = 17.0 \times 10^{11} cm^{-2}$, a value that our results show to be too large. Fitting a Gaussian H-F obtained, for $N_{ox} = 3.5 \times 10^{11} cm^{-2}$ the maximum of the DOS equal to $3.4 \times 10^{13} cm^{-2} eV^{-1}$ and a bandwidth $\Gamma = 1.8 meV$. Our calculations give, taking into account the double degeneracy of the first subband, $D(E)_{max} = 2.32 \times 10^{13} cm^{-2} eV^{-1}$ and a dispersion $\Gamma = 5.1 meV$. The last value is in disagreement mainly because the shape of the band is very asymmetric and a Gaussian becomes a very poor approximation. In addition, it is important to mention some uncertainty in the experimental data available[14].

Finally, we have investigated the effect of the applied field (or N_{depl}) in the DOS. The results are shown in Fig. 3 for the bandwidth (dispersion in the lower subband) and the energy of the maximum DOS. In Fig. 3a we observe the broadening of the impurity band with the increase of the electric field. This effect has, in fact, been observed by H.F. As shown in Fig. 3b, the position of the maximum of the DOS goes to higher energies as N_{depl} increases. In both Figs. we can observe that increasing the impurity concentration results in enhancing the effect of the applied field.

REFERENCES

[1]T. Ando, A.B. Fowler, F. Stern; Rev. of Modern Phys. 54, 437 (1982).

[2]A. Hartstein and A.B. Fowler; Phys. Rev. Lett. 34, 1435 (1975).
A.B. Fowler and A. Hartstein; Phil. Mag. B 42, 949 (1980).

[3]E. Glaser, R. Czaputa, B.D. McCombe, G.M. Kramer and R.F. Wallis; Phys. Rev. Lett. 57, 843 (1986).

[4]F. Stern and W.E. Howard; Phys. Rev. 163, 816 (1967).

[5]B.G. Martin and R.F. Wallis; Phys. Rev. B 18, 5644 (1978).

[6]N.O. Lipari; J. Vac. Sci. Technol. 15, 1412 (1978).

[7]B. Vinter; Phys. Rev. B 26, 6808 (1982).

[8]I.C. da Cunha Lima, A. Ferreira da Silva, P.S. Guimarães, L.F. Perondi and J.R. Senna; Phys. Rev. B 32, 2371 (1985).

[9]R. Kishore; Phys. Rev. B 19, 3822 (1979).

[10]A. Ferreira da Silva, R. Kishore and I.C. da Cunha Lima; Phys. Rev. B 23, 4035 (1981).

[11]T. Matsubara and Y. Toyozawa; Prog. Theor. Phys. 26, 739 (1961).

[12]I.C. da Cunha Lima and A. Ferreira da Silva; Phys. Rev. B 30, 4819 (1984).

[13]The electron-electron interaction potential $V(\vec{r}_1,\vec{r}_2)$ used is that given by Eq. (2.50) of Ref. 1.

[14]A. Hartstein and A.B. Fowler; Bull. Am. Phys. Soc. 28, 322 (1983).

FIGURE CAPTIONS

Fig. 1 - Correlation energy U as a function of the applied electric field.

Fig. 2 - The calculated density of impurity states: Dotted line gives the energy of the single-impurity ground state; dashed lines give the minimum of the first unperturbed subband.

Fig. 3 - The dispersion Γ and the energy of maximum DOS of the lower Hubbard band as a function of impurity concentration.

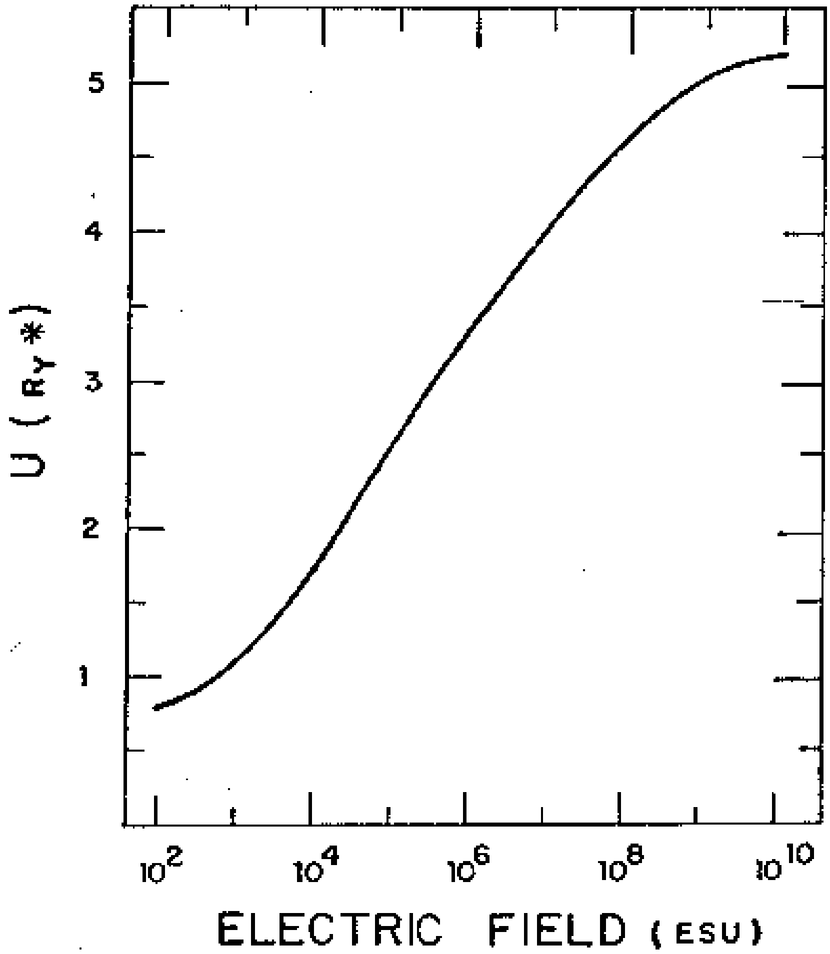

Figure 1 - Andrada e Silva and da Cunha Lima

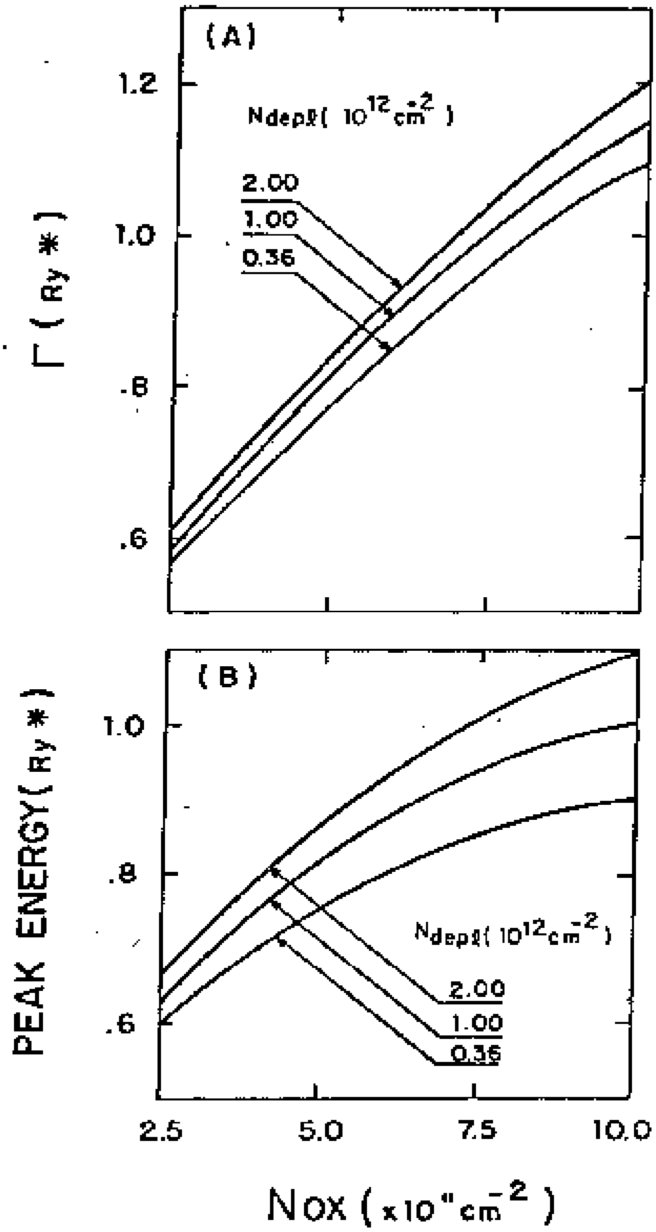

Figure 3 - Andrada e Silva and da Cunha Lima

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