1. Publication Nº	2. Version	3. Date	5. Distribution
INPE-2996-PRE/448	*2nd	Feb., 1984	☐ Internal ☒ External ☐ Restricted

4. Origin: DTE/DCT — Program: MATERIALS

6. Key words - selected by the author(s)

INVERSION LAYERS
2D IMPURITY HUBBARD BANDS
HERERO-STRUCTURE INTERFACES

7. U.D.C.: 539.2

8. Title: INPE-2996-PRE/448

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10. Nº of pages: 12

11. Last page: 10

12. Revised by

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Director General

14. Abstract/Notes

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15. Remarks

This paper will be submitted to Physical Review B.
*2nd revised version, April 1984.

TWO-DIMENSIONAL IMPURITY BANDS AT SEMICONDUCTOR HETERO-STRUCTURE INTERFACES

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ABSTRACT

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.

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

We assume a Hubbard-like Hamiltonian

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

where $a^{+}_{i\sigma}$ 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 $n_{i\sigma} = a^{+}_{i\sigma}\, a_{i\sigma}$. 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

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

and

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

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] (M-T) theory for doped semiconductors. It seems to be a general property of tight-binding Hamiltonians for regular 2-D 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 M-T theory is very convenient to obtain information about those properties in the case of 2-D 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 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] (S-H) using the effective-mass theorem and considering a thickless inversion-layer, many improvements have been achieved[5].

Our present calculations of impurity bands correspond to the rather unrealistic case of the S-H solution for the bound state with unscreened impurity potential and with the impurity located itself at the inversion layer. This rough treatment generates 2-D hydrogen-like bound states with binding energy equal to 4 Ry*. Although this over-simplification 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

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

where a_0 is the effective Bohr radius, $a_0 = \bar{k}h/m^*e^2$ and $\bar{k} = (k_{ox} + k_{Si})/2$. For the case of $Si-SiO_2$, 1Ry* = 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 2-D case. We define two Green's functions, $G^{+}_{ij\sigma}$ and $G^{-}_{ij\sigma}$ as

$$G^{\pm}_{ij\sigma}(t) = - i\theta(t) < [a_{i\sigma} n^{\pm}_{i-\sigma}, a^{+}_{j\sigma}(t)]_{+} > , \tag{5}$$

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

$$<G^{\pm}_{ii\sigma}(w)>_{av} = \frac{n^{\pm}_{-\sigma}}{w-E^{\pm}} \xi^{\pm}(w-E^{\pm}) , \tag{6}$$

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

$$\xi^{\pm}(w) = 1 + \frac{<V_{ii}>_{av}}{w-E^{\pm}} + \frac{<\Sigma_l V_{il} V_{li}>_{av}}{(w-E^{\pm})^2} + \ldots \tag{7}$$

In 2-D, ξ obeys the equation

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

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

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:

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

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

$$w < G_{ii\sigma}(w) > \; = n_{-\sigma}^{-} \; \xi(w) \; . \tag{11}$$

Defining

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

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

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

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

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

and

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

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

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

In the above notation

$$\mathrm{Re} < G_{ii}(w) > = \frac{1}{Na_0^2} \cdot \frac{u}{u^2 + s^2} \tag{16}$$

and

$$\mathrm{Im} < G_{ii}(w) > = -\frac{1}{Na_0^2} \cdot \frac{u}{u^2 + s^2} \, . \tag{17}$$

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

$$s(w) = 0 \quad \text{for} \quad E_\ell > w \quad \text{or} \quad w > E_u,$$
$$u(w) \to 0 \quad \text{as} \quad w \to E_\ell^- \quad \text{or} \quad w \to E_u^+.$$

Bringing these results into Eq. (17) we see that the discontinuities lead to the unphysical result of $E_\ell = E_u = V(R = 0)$. 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--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 $V(x) = -8x\ K_1(x)$ 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

$$V(k) = - \frac{128\pi\, a_o^2}{(4 + a_o^2 k^2)^2} \text{ Ry*}. \qquad (18)$$

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 $6.20 \times 10^{11} cm^{-2}$.

It is evident that no discontinuity is observed on the band edges. However, a band tail pointing to the low energy region characteristic of impurity bands in 3-D is not observed in 2-D bands. This feature does not seem to be a result of the approximation involved in the M-T 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 they 2-D energy bands.

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

REFERENCES

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

[2]E.N. Economou, Green's Function in Quantum Physics (Springer, Berlin, 1979).

[3]A. Hartstein and A.B. Fowler, in Proceedings of the 13th International Conference on the Physics of Semiconductors, Rome, 1976, edited by F.G. Fermi, p. 741.

[4]F. Stern and W.E. Howard, Phys. Rev. 163, 826 (1967).

[5]See, e.g., T. Ando, A.B. Fowler and F. Stern, Rev.Mod. Phys. 54, 437 (1982), and references therein.

[6]A. Ferreira da Silva, R. Kishore and I.C. da Cunha Lima, Phys. Rev. B23, 4035 (1981); R. Kishore, I.C. da Cunha Lima, M. Fabbri and A. Ferreira da Silva, Phys. Rev. B26, 1038 (1982).

[7]L.F. Perondi (unpublished).

[8]I.C. da Cunha Lima, A. Ferreira da Silva and M. Fabbri, Surf. Sci. 134, 235 (1983).

[9]A. Puri and T. Odagaki, Phys. Rev. B24, 5541 (1981).

FIGURE CAPTIONS

Fig. 1 - Top and bottom edges of the 2-D 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_o 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 overlaping.

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_o.

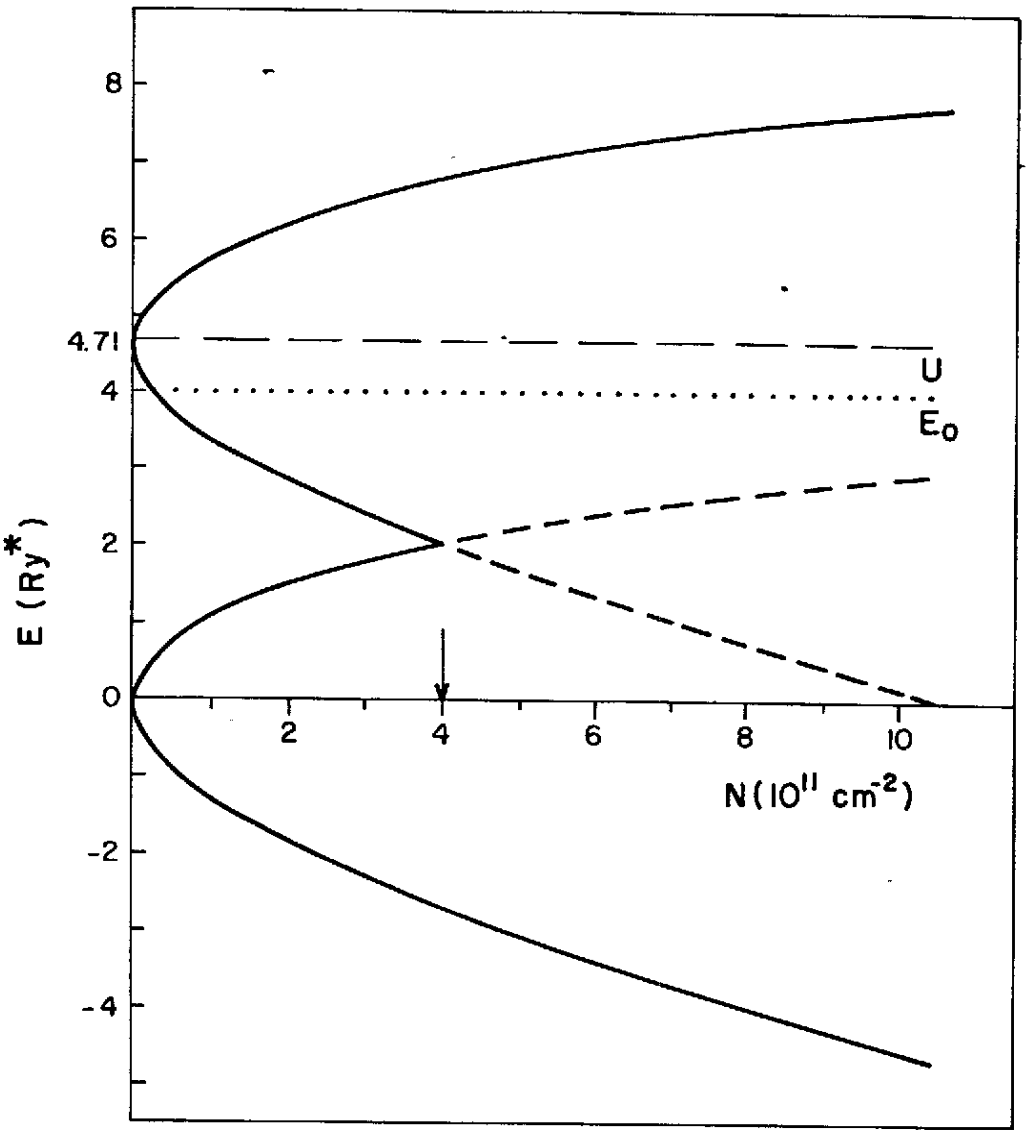

Fig. 1 - I.C. da Cunha Lima and A. Ferreira da Silva

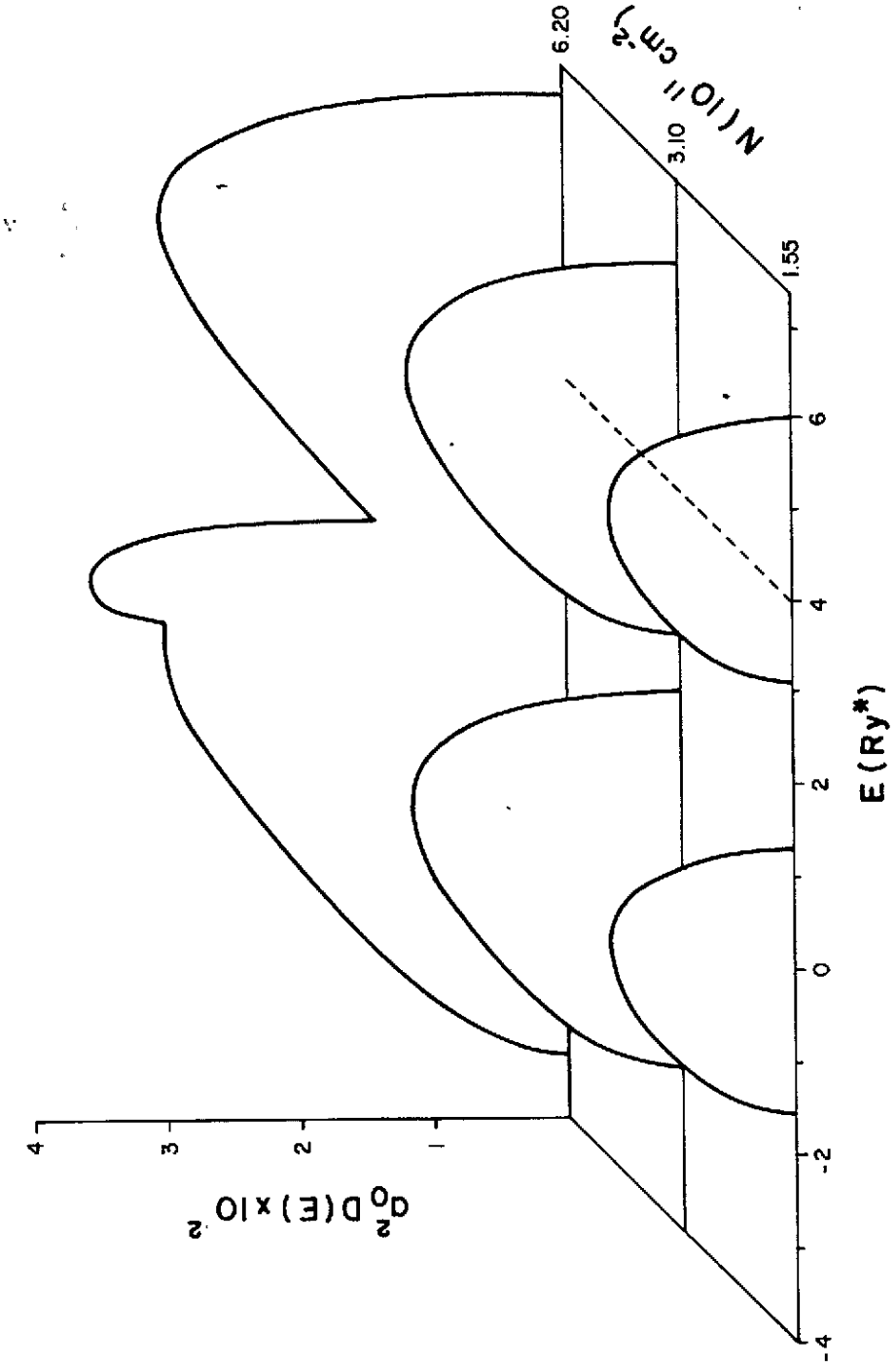

Fig. 2 - I.C. da Cunha Lima and A. Ferreira da Silva