

1. Publication Nº <i>INPE-3447-PRE/700</i>	2. Version	3. Date <i>March, 1985</i>	5. Distribution <input type="checkbox"/> Internal <input checked="" type="checkbox"/> External <input type="checkbox"/> Restricted
4. Origin <i>DTE</i>	Program <i>MATER</i>		
6. Key words - selected by the author(s) <i>IMPURITY CLUSTER STATES</i> <i>DOUBLE DONOR SYSTEM</i> <i>SIMULATION</i>			
7. U.D.C.: <i>539.2</i>			
8. Title <i>INPE-3447-PRE/700</i> <i>ELECTRONIC DENSITY OF STATES FOR THE</i> <i>DOUBLE DONOR SYSTEM Si:P, As</i>		10. Nº of pages: <i>11</i>	11. Last page: <i>10</i>
9. Authorship <i>A. Ferreira da Silva</i> <i>M. Fabbri</i>		12. Revised by <i>Ram Kishore</i> <i>Ram Kishore</i>	
Responsible author <i>A.F.S.</i>		13. Authorized by <i>Parada</i> <i>Nelson de Jesus Parada</i> <i>Director General</i>	
14. Abstract/Notes <i>We investigate the tight-binding bands arisen in the one-electron, effective-mass approximation of the Si:P, As system by a computer simulation, which is carried out with a double hydrogenic 1s basis with proper Bohr radii and ionization energies. In the low concentration regime, the effect of the additional vertical disorder appears to be not sensitive to the relative amount of As and P atoms. The space-filling argument of Newman and Holcomb is confirmed in the region near the metal to non-metal transition.</i>			
15. Remarks <i>This paper will be submitted to publication in the Revista Brasileira de Física (Special Issue) of the II Escola Brasileira de Física de S̄ēmicondutores.</i>			

ELECTRONIC DENSITY OF STATES FOR THE
DOUBLE DONOR SYSTEM Si: P, As

A. Ferreira da Silva and M. Fabbri

Instituto de Pesquisas Espaciais - INPE
Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPq
12200 São José dos Campos - SP - Brasil

We investigate the tight-binding bands arisen in the one-electron, effective-mass approximation of the Si: P, As system by a computer simulation, which is carried out with a double hydrogenic $1s$ basis with proper Bohr radii and ionization energies. In the low concentration regime, the effect of the additional vertical disorder appears to be not sensitive to the relative amount of As and P atoms. The space-filling argument of Newman and Holcomb is confirmed in the region near the metal to non-metal transition.

I. INTRODUCTION

Recently, the double donor system Si: P, As was investigated both experimentally and theoretically by Newman and Holcomb (NH)⁽¹⁾. They found that the experimental result for n_c , the critical concentration for the metal to non-metal transition, can be explained by a simple scale argument, based only in the space filling by the two types of donors (P, As) with different Bohr radii. They also stressed the fact that this behaviour is expected if one neglects the additional vertical disorder introduced by the different single-site ionization energies in the double donor system, as compared with the single donor systems Si:P and Si:As. Their findings motivated us to do a computer simulation with a finite cluster for the double donor system along the lines of our previous works with Si:P⁽²⁾. In its simplest version, these cluster models neglect diagonal disorder, and works with a tight-binding (LCAO) approach with a basis of hydrogenic 1s functions at the impurity sites; electron-electron correlations are also disregarded. Therefore, this oversimplified model meets all the conditions found in Newman and Holcomb works; in particular, they supposed that the diagonal disorder due to the statistical spread of the single-site ionization energies in any of the single systems Si:P or Si:As is much less than the difference in the ionization energies between P sites and As sites, at the concentrations of interest.

II. DESCRIPTION OF THE MODEL

We generate M sites following a Poisson process over the surface of a four-dimensional sphere of radius $R^{(3)}$, in a way to incorporate periodic boundary conditions. Employing the dimensionless impurity concentration

$$P = 32\pi n a_H^{*3} , \quad (1)$$

where n is the true concentration and a_H^* is the effective Bohr radius, the radius R must be, then,

$$R = \left(\frac{16M}{\pi P} \right)^{1/3} . \quad (2)$$

In order to maintain close resemblance with the three-dimensional cluster, we have $R \gg R_0$, where R_0 is the range of the potentials involved or the related matrix elements.

In a fraction q of these M sites we put As atoms, and in the remaining $(1-q)M$ sites we put P atoms. For the scaling argument we employ the reduced concentration introduced by NH

$$\eta = \frac{n_P}{(n_c)_P} + \frac{n_{As}}{(n_c)_{As}} , \quad (3)$$

where n_P is the concentration of P atoms and $(n_c)_P$ is the critical concentration for the Si:P system; the second term is the same ratio for As atoms. We see that the scaling argument applies when a physical property shows the same behaviour with η for all the similar systems. NH verified that this is the case for the conductivity near $\eta \sim 1$.

The cluster Hamiltonian of the system, only for the electron-ion interactions, is

$$H = \sum_{i=1}^M h_i \quad (4)$$

$$h_i = - \frac{\nabla_i^2}{2} - \sum_j \frac{1}{r_{ij}} , \quad (5)$$

where r_{ij} is the position of the i -th electron relative to the j -th site. The sample is supposed uncompensated. The eigenfunctions are restricted to the LCAO class

$$\psi_i(r) = \sum_{j=1}^M c_{ij} \phi_j(r) , \quad (6)$$

where $\phi_j(r)$ is a 1s hydrogenic function centered at the j-th site, with appropriate Bohr radius. Inserting (6) in (5) and disregarding terms corresponding to ionic diagonal attraction and three-center integrals, we get the Hamiltonian matrix

$$H_{ij} = \begin{cases} E_D^i & \text{if } i=j \\ V_{ij} & \text{if } i \neq j \end{cases}, \quad (7)$$

where E_D^i is the ionization energy for the corresponding sites and

$$V_{ij} = \langle \phi_i | \frac{-1}{|\vec{r} - \vec{R}_j|} | \phi_j \rangle \quad (8)$$

are the hopping terms.

Since we are not here interested in the detailed behaviour of the matrix elements, we disregard overlap terms in (7) and in the diagonalization of the Hamiltonian. The full expression for the hopping matrix V_{ij} is

$$V_{ij}(R) = \frac{(\alpha\beta)^{1/2}(w^2-v^2)}{2w^2v^2} e^{-w} \{ (e^V - e^{-V})(w+v) - 2wve^{-V} \}, \quad (9)$$

where

$$w = \frac{\alpha+\beta}{2} R$$

and

$$v = \frac{\alpha-\beta}{2} R .$$

The parameters α and β come from

$$\phi_i(r) = \sqrt{\frac{\alpha^3}{\pi}} e^{-\alpha r}$$

and

$$\phi_j(r) = \sqrt{\frac{\beta^3}{\pi}} e^{-\beta r} .$$

For $\alpha=\beta$, we get the usual hopping between two hydrogenic centers of the same radii, at a distance R apart

$$V_{ij}(R) = -e^{-\alpha R}(1+\alpha R) . \quad (10)$$

$\alpha \rightarrow \beta$

Note that $V_{ij}(R)$ is not symmetric with an interchange of α and β ; in order to keep (7) Hermitian, we choose only the As-P type of hopping for either a As-P or a P-As pair (this difference would be naturally compensated if we had taken the overlap terms into account; but this approximation is not crucial at this level of the calculation).

Naturally, when $\alpha \gg \beta$, or vice versa, we get $V_{ij} \rightarrow 0$; this is due to the fact that in this case the two impurity systems could be treated separately.

In order to study the physical behaviour of the spatial distribution of the eigenvectors, which we think is in our model the feature most closely related to the conductivity in the real system, we have used the Inverse Participation Ratio (IPR)⁽²⁾ for each eigenvector

$$(IPR)_i = \frac{\sum_{j=1}^M |c_{ij}|^4}{\left[\sum_{j=1}^M |c_{ij}|^2 \right]^2} , \quad (11)$$

where c_{ij} comes from Eq. (6). The IPR's range from 1 to $1/M$, corresponding to a completely localized state (around one impurity) to

a state covering all the cluster extension. As we stressed in a previous work⁽²⁾, this quantity is not directly related to localization in real space (and to be sure, neither our finite cluster calculation), but we expect that, if the scale argument turns out to hold for these clusters, we have no reason to expect the contrary in the real system (the converse being not true).

III. RESULTS

We have used the IPR values of the eigenvectors for a Poisson cluster of $M = 80$ impurities, with a number of $qM = 80, 60, 40$ and 0 As atoms and the remaining quantity of P atoms. The As and P atoms were simulated by single hydrogenic $1s$ functions with different Bohr radii and corresponding ionization energies, i.e.,

$$\begin{aligned}\alpha &= 1, \text{ for P atoms,} \\ \beta &= 1.2 \text{ (As atoms),} \\ E_D^1 &= -1.0 \text{ Ry}^* \text{ (P atoms),} \\ E_D^2 &= -1.44 \text{ Ry}^* \text{ (As atoms).}\end{aligned}\tag{12}$$

The unit of energy is the effective Rydberg, and the Bohr radius for P atoms was taken equal to 1. The value $\beta = 1.2$ for As atoms we got from the relation of the two Bohr radii from NH; in this simple hydrogenic model, the Bohr radius goes with $1/\alpha$ and the ionization energy with α^2 (of course this is only a crude estimation for the real system, the chemical shift is not playing a central role in our model).

In order to study scaling behaviour, we used the same cluster for all concentrations of interest; only a multiplicative scale factor in the coordinates was employed to adjust the concentration value.

For each reduced concentration, we calculated the mean value of the IPR ($\langle \text{IPR} \rangle$) ratio for all eigenvectors. The results are shown in Fig. 1. We note that the argument of NH is confirmed for the region $\eta > 1$, the additional vertical disorder bringing no change in

the qualitative behaviour of the eigenvectors. For low concentrations, on the contrary, this small amount of vertical disorder enhances the localization of the eigenstates, and it is not a trivial result that, for different amounts of As atoms, we get again the same qualitative behaviour (curves for $q = 0.5$ and 0.75). A more detailed study will be reported briefly.

REFERENCES

- (1) P.F. Newman and D.F. Holcomb, Phys. Rev. Lett. 51 2144 (1983);
Phys. Rev. B28 638 (1983).
- (2) M. Fabbri and A. Ferreira da Silva, J.Non-Cryst. Solids 55 103
(1983); *ibid*, Phys. Rev. B29 5764 (1984); A. Ferreira da Silva
(this issue).
- (3) M. Fabbri (this issue).

FIGURE CAPTION

Fig. 1 - $\langle IPR \rangle$ For various values of the reduced concentration η , and for different amount of As atoms; full circles denote $q = 0$ (80 P-atoms), open circles $q = 1$ (80 As-atoms), full triangles $q = 0.75$ (60 As-atoms and 20 P-atoms), open triangles $q = 0.5$ (40 As-atoms and 40 P-atoms).

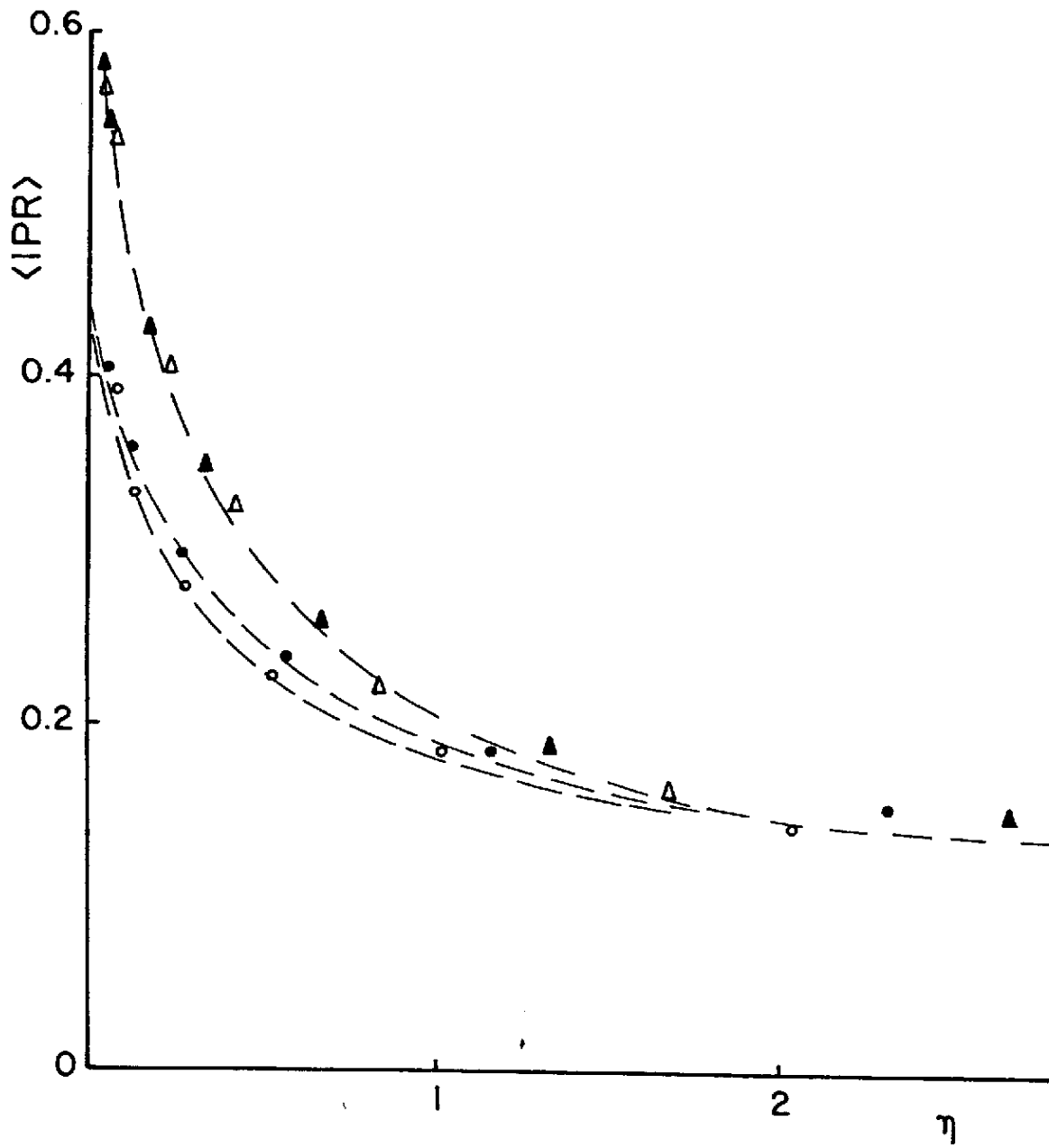


Fig. 1 - A. Ferreira da Silva and M. Fabbri