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14. Abstract/Notes <p><i>We investigate the microscopic structure of the impurity states in two-and three-dimensional (2D and 3D) disordered systems. A cluster model is outlined for the donor impurity density of states (DIDS) of doped semiconductors. It is shown that the impurity states are very sensitive to a change in the dimensionality of the system, i.e., from 3D to 2D system. It is found that all eigenstates become localized in 2D disordered system for a large range of concentration.</i></p>			
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IMPURITY STATES IN TWO-AND THREE-DIMENSIONAL DISORDERED SYSTEMS

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ABSTRACT

We investigate the microscopic structure of the impurity states in two-and three-dimensional (2D and 3D) disordered systems. A cluster model is outlined for the donor impurity density of states (DIDS) of doped semiconductors. It is shown that the impurity states are very sensitive to a change in the dimensionality of the system, i.e., from 3D to 2D system. It is found that all eigenstates become localized in 2D disordered system for a large range of concentration.

Impurity states in 2D and 3D systems have attracted considerable interest, because of the existence of the poorly understood metal-nonmetal (MNM) transition in doped semiconductors. The commonly used approaches in the theoretical investigations of such systems are based on the very well-known Mott-Hubbard-Anderson model¹. In this model the electron correlation and the Anderson localization are regarded as the most essential factors, and the DIDS is split into two Hubbard bands, situated within the band gap of the host material. These two bands are identified as the lower (D^0 -singly occupied impurities) and the upper (D^- -doubly occupied impurities) Hubbard bands, separated by the intra-atomic Coulomb correlation energy U^2 . The correlation

effect is seen in the D^- state through the formation of stable bound state, found experimentally by Narita and co-workers³. With increasing impurity concentration, these bands broaden and eventually start overlapping each other as well as with those corresponding to the host material.

The purpose of this work is mainly to investigate the influence of the impurity states in disordered systems, when the dimensionality is changed from three to two dimensions. Recently, the present authors⁴, by employing a simple one-electron Hamiltonian for the 2D case, found a symmetric impurity band with a considerable bandwidth for high concentration, while for low concentration it is drastically reduced by the cut-off of the long-range hopping energy. Here, as we will see later, we perform an improved self-consistent cluster calculation with spin-polarized potentials. We assume the bound state as a hydrogenic wavefunction in 2D⁴, in the light of the work in inversion layer by Stern and Howard⁵, who carried out a calculation for an inscreened impurity located at the inversion layer, assumed as widthless sheet⁶. We show, in Fig. 1, for the sake of comparison, the charge density of both 2D and 3D wavefunctions.

For a given impurity concentration N , we generate a cluster of M random sites $\{\vec{R}_i; i=1, M\}$ in a square of length L (volume Ω of a diamond lattice host), representing the location of M substitutional impurities. Thus, we simulate a sample of 2D (3D) disordered system. With each impurity is associated a wavefunction $\psi_i(\vec{r})^\gamma$, where $\gamma = 2D$ or 3D. The Hamiltonian of such system with M electrons is

$$H = \sum_i \frac{p_i^2}{2m} + \sum_i V^{\text{ion}}(\vec{r}_i) + \frac{1}{2} \sum_{i,j} V^{\text{el-el}}(\vec{r}_i, -\vec{r}_j), \quad (1)$$

where $V^{\text{ion}}(\vec{r}_i)$ is the impurity -ion potential acting on the i -th electron, $V^{\text{el-el}}(\vec{r}_i, -\vec{r}_j)$ is the Coulomb interaction between the i -th and j -th electron, and the summation are over all the M electrons in the square L (volume Ω). The Hamiltonian will be solved with the Unrestricted Hartree-Fock-Roothaan (UHFR) formalism with spin-polarized potential⁷ which was developed earlier by Fabbri and Ferreira da Silva⁷ to take the problem of multi-valley⁸ effects in doped semiconductors. Here we will only outline the key points. The UHFR equations are given by the following sets of coupled Schrödinger equations,

$$H_{\text{O}\sigma}(\vec{r}) \psi_{n\sigma}(\vec{r}) = E_{n\sigma} \psi_n(\vec{r}), \quad \sigma = \uparrow, \downarrow \text{ and } n = 1, M, \quad (2)$$

where

$$H_{\text{O}\sigma}(\vec{r}) = \frac{p^2}{2m} + V^{\text{ion}}(\vec{r}) + V_{\sigma}^{\text{Coul}}(\vec{r}) + V^{\text{Exch}}(\vec{r}). \quad (3)$$

The single-particle eigenfunction can be constructed from the set of localized orbitals $\psi_j(r)^Y$, as

$$\psi_{n\sigma}(\vec{r}) = \sum_j \psi_j(\vec{r})^Y B_{jn\sigma}. \quad (4)$$

Then, the UHFR procedure leads to two coupled M by M matrix equations for both spin $\sigma = \uparrow$ and \downarrow :

$$\sum_j [\bar{B}_{\sigma}^{\dagger} \bar{H}_{\text{O}\sigma} \bar{B}_{\sigma}]_{ij} - E_{m\sigma} \delta_{ij} C_{mj\sigma} = 0, \quad (5)$$

where \bar{B}_{σ} is the matrix of the coefficients $B_{\sigma ij}$ and $E_{m\sigma}$ is the diagonal UHFR eigenenergy matrix for the spin σ . After solving (5), in terms of

the Slater integrals, the DIDS $D(E)$ can be easily computed and normalized to

$$\int D(E) dE = \frac{P}{64\pi} = \left(\frac{M}{L}\right) a_H^2, \quad (6)$$

in two dimensions, and

$$\int D(E) dE = \frac{P'}{32\pi} = \left(\frac{M}{\Omega}\right) a_H^3, \quad (7)$$

in three dimensions, where a_H is the effective Bohr radius. The constants 64π in 2D and 32π in 3D were chosen only for convenience. In our calculation we use $M = 40$ impurities, surrounded by 960 impurities forming an effective field, and so avoiding surface effects⁷. The configuration average is taken over 50 samples when the self-compensation effects⁷ is not taken into account. The 2D DIDS is shown in Fig. 2 as a function of the dimensionless impurity concentration P .

To study the character of the eigenstate we have calculated the inverse participation ratio (IPR)^{7,8}

$$L_{n\sigma} = \left(\sum_j |B_{jn\sigma}|^4\right) / \left(\sum_j |B_{jn\sigma}|^2\right)^2, \quad (8)$$

for each eigenstate $\psi_{n\sigma}(\vec{r})$. These are calculated as a function of eigenenergy for different impurity concentrations (dots in Fig. 2). For small P most of the states have an IPR between 0.5 and 1.0, indicating an isolated impurity state or a pair state in agreement with the conclusions, in 3D system, reached by Thomras et al.⁹, through their analysis of optical data. In the intermediate regime, larger cluster become more abundant and the one-particle eigenstate are

localized on cluster of variable sizes. In the metallic regime (high concentration), still a non-negligible fraction of the occupied states shows localized character. In Fig. 3 we show the configuration average $\langle L_{n\sigma} \rangle$'s from low to intermediate regime of concentration, for both 2D and 3D systems. We can see that, in two dimensions, the $\langle L_{n\sigma} \rangle$ is greater than 0.5 for all range of concentration presented here. It shows that, for two dimensions the system is composed by isolated impurities or pair of impurities, while for the 3D case the system passes from localized to extended states. This finding indicates that all eigenstates become localized for such 2D disordered system, contrary to the 3D system. A more complete discussion (and calculation) about the existence or nonexistence of extended electronic states in 2D disordered systems are in progress and will be reported elsewhere.

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FIGURE CAPITIONS

Fig. 1 - Charge density for 2D and 3D systems.

Fig. 2 - 2D DIDS for $P = 12(N^{1/2}a_H = 0.24,)$. It corresponds to $N = 2.0 \times 10^{12} \text{ cm}^{-2}$, with $a_H = 17.3 \text{ \AA}$. The dots correspond to the IPR. The arrow indicates E_F . Shaded area represents the overlap of split bands. The host material is set at zero energy. The ionization energy, set at the lower D^0 band, is -2.0 Hartrees.

Fig. 3 - $\langle L_{n\sigma} \rangle \equiv \langle \text{IPR} \rangle$ for various values of the impurity concentration $P(2D)$ and $P'(3D)$. For comparison $P' = 1.0$ ($N^{1/3}a_H = 0.21$, Mott's relation), corresponds to $N = 1.9 \times 10^{18} \text{ cm}^{-3}$, $P = 16$ ($N^{1/2}a_H = 0.28$) corresponds to $2.66 \times 10^{12} \text{ cm}^{-2}$. The dots represent the individual $L_{n\sigma}$, in 2D case, for each configurations, at a fixed P .

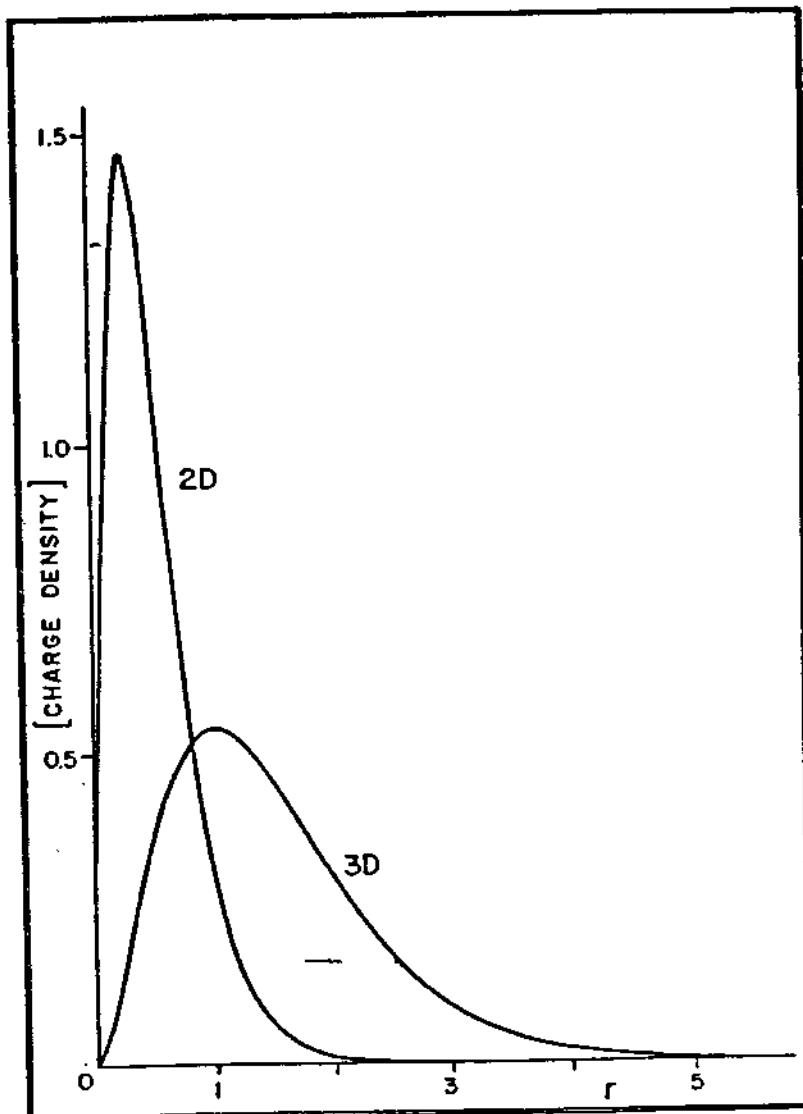


Fig. 1 A. Ferreira da Silva and M. Fabbri

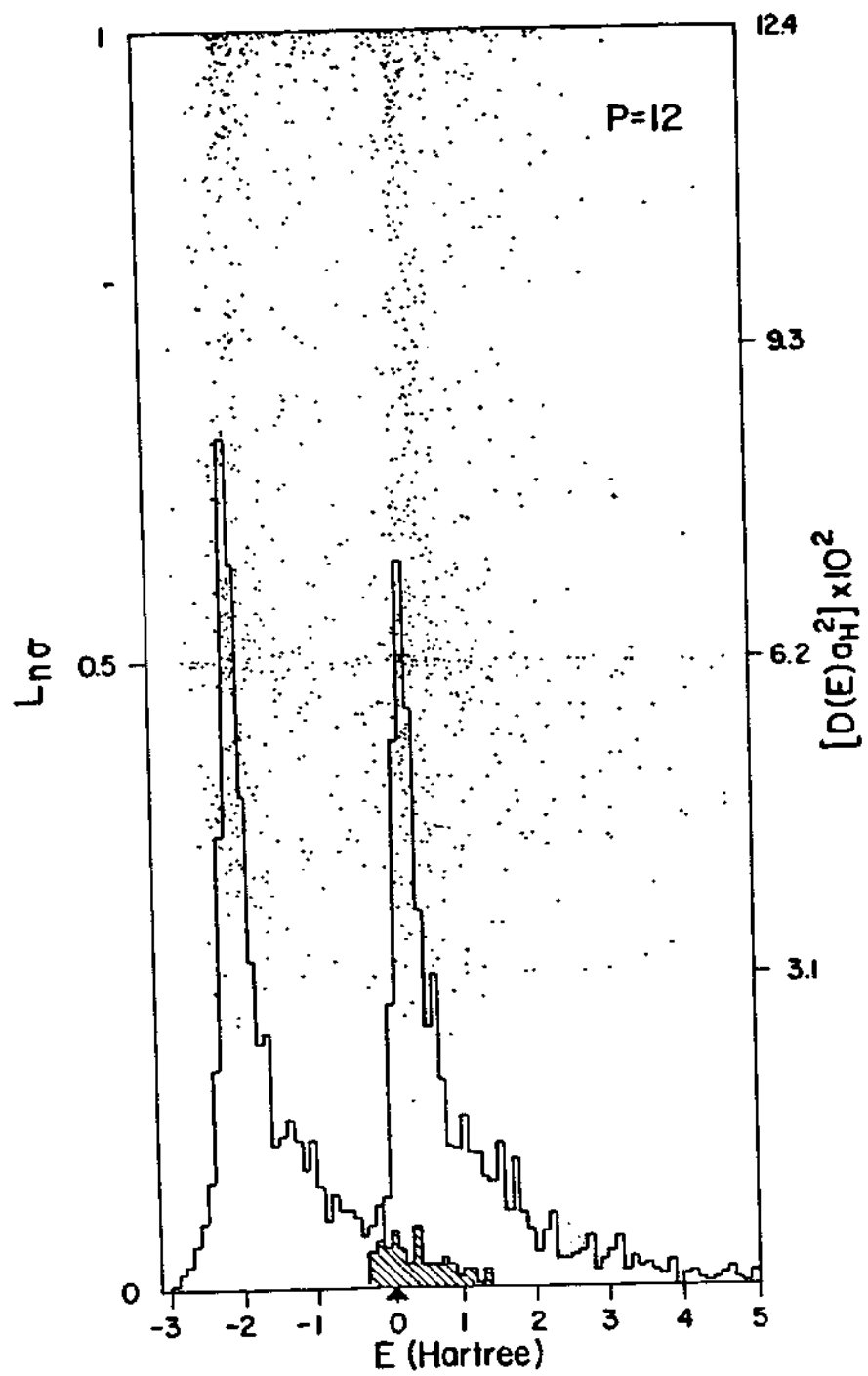


Fig. 2 A. Ferreira da Silva and M. Fabb

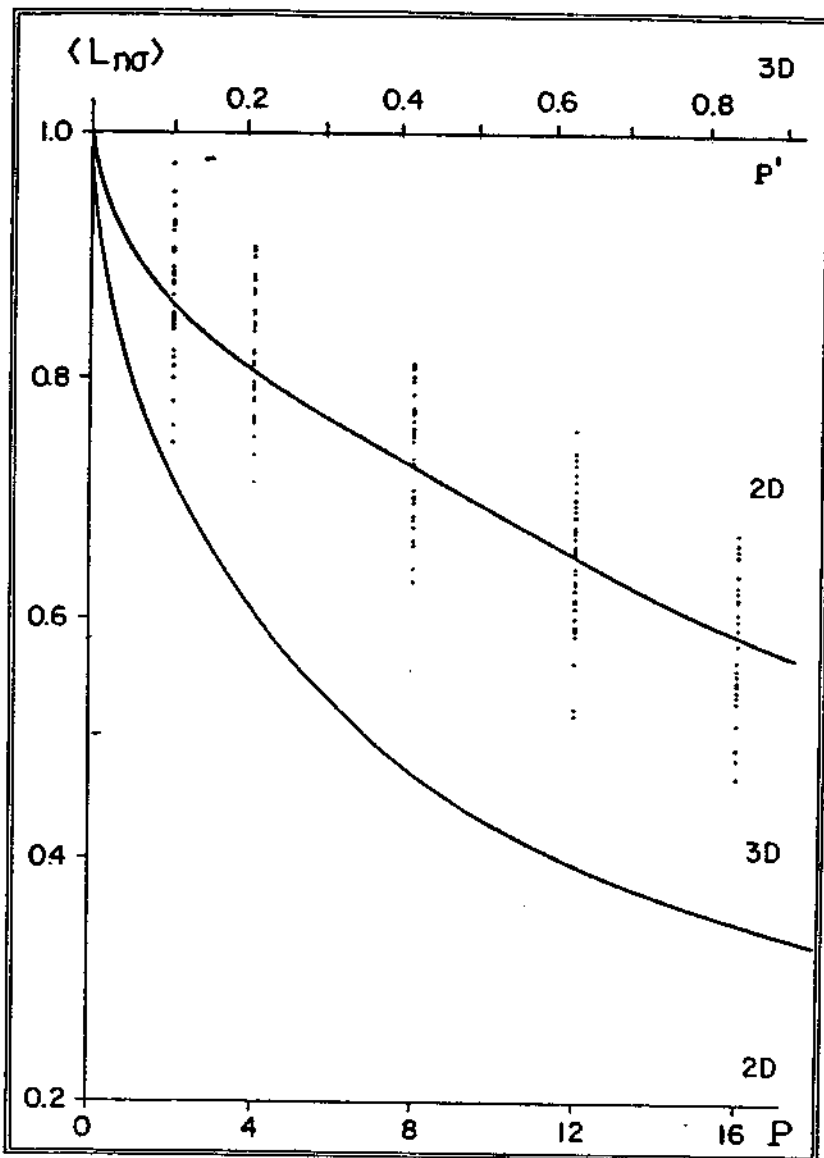


Fig. 3 A. Ferreira da Silva and M. Fabbri