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# Impurity states in a quantum-well wire of GaAs-$Ga_{1-x}Al_xAs$

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We investigate the behavior of the hydrogenlike impurity states in a small wire of GaAs inside a $Ga_{1-x}Al_xAs$ structure. The effects of disorder are taken into account in the calculation. It is shown that the hopping energy plays an essential role in the formation of the impurity bands and that the peak energy as a function of impurity concentration or wire dimension behaves in the same way for both cases. Results are compared to a recent experiment on cathodoluminescence.

It is very well known that impurity bands have important consequences in optical studies and transport measurements on small semiconductor structures such as heterostructure, quantum wells, and quantum-well wires (QWW's). This has recently been a very active field of research,[1-9] motivated largely by the development of molecular-beam epitaxy and metal-organic chemical-vapor deposition techniques which have made it possible to fabricate high-mobility semiconductor microstructures with extremely small spatial extensions.[3,10,11] Here we will focus on a QWW that is made of GaAs, which is surrounded by $Ga_{1-x}Al_xAs$, and has a square cross section of width $L$. In this heterojunction the electronic motion is quantum-mechanically confined on the plane $XY$ while being free to move in the $Z$ direction, along which quasi-one-dimensional (quasi-1D) transport can occur. In the wake of previous calculations done for a QWW,[12] we assume the Hamiltonian in a random, one-body tight-binding approximation, with monovalent impurities as

$$H=E_B\sum_i |i\rangle\langle i|+\sum_{i\neq j} V_{ij}|i\rangle\langle j| \ , \tag{1}$$

where $E_B$ is the binding energy, which is taken as our energy origin, $V_{ij}$ is the random energy integral for the transfer of an electron from the $i$th site to the $j$th site (i.e., hopping matrix), and $\langle \mathbf{r}|i\rangle=\Psi(\mathbf{r}-\mathbf{R}_i)$ is the ground-state wave function of an electron bound to an impurity at $\mathbf{R}_i$. The impurity bandwidths and the density of states D(E) are calculated from the Green's functions

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

with configuration averaging over the random distribution of impurities. We treat this configurational average according to the Matsubara-Toyozawa (MT) (Ref. 13) theory for doped semiconductors. Let us define

$$\xi^{(\pm)}(\omega)=Z_\pm\langle G_{ii}^{(\pm)}(\omega)\rangle \ , \tag{3}$$

where $\langle\cdots\rangle$ means configuration averaging and $Z_\pm=\omega\pm i\varepsilon$. As the impurities are distributed completely at random, the configuration average can be performed by making the positions of all intermediate impurity sites that appear in the Green's function run over the whole space with equal probability. If the summation over intermediate impurity sites is replaced by an integral, $\sum_i\rightarrow N\int d\mathbf{R}_i$, where $N$ is the impurity concentration, one can then obtain

$$Z^\pm\langle G_{ij}^{(\pm)}(\omega)\rangle=\delta_{ij}+\frac{V_{ij}}{Z_\pm}+\sum_{\nu=1}^{\infty}\sum_{\mu=1}^{\nu}\frac{N^\mu}{Z_\pm^{\nu+1}}\int dR_1\cdots\int dR_\mu V(R_{\mu\rho 1})V(R_{\rho 1,\rho 2})\cdots V(R_{\rho\nu\mu}) \ . \tag{4}$$

For a given value of $Z$ (from now on we will omit the symbols $\pm$), those terms with smaller $\nu$-$\mu$ values make larger contributions when $N$ is large. Following this leading principle, MT have chosen only those diagrams in which different journeys have no common sites with one another. The coupled equations derived from this scheme are written, in our 1D version, as

$$\xi=(1-\eta)^{-1} \ , \tag{5}$$

$$\eta=1-\frac{1}{\xi(\omega)}=\frac{N\xi(\omega)}{2\pi\omega^2}\int\frac{V^2(\mathbf{k})dk}{1-N\xi(\omega)/V(\mathbf{k})\omega} \ . \tag{6}$$

In the above equation $N$ is the number of impurities per cm and $V(\mathbf{k})$ is the 1D Fourier transform of hopping energy $V_{ij}=V(\mathbf{R}_i-\mathbf{R}_j)=V(z)$:

$$V(k)=\int\exp(ikz)V(z)dz \ . \tag{7}$$

Defining

$$\frac{\xi(\omega)}{\omega}=\{Na_0^*[u(\omega)+is(\omega)]\}^{-1} \ , \tag{8}$$

where $a_0^*$ is the effective Bohr radius, we have for the density of states $D(\omega)$

$$D(\omega)=\frac{-1}{\pi}\text{Im}\left[\frac{\xi(\omega)}{\omega}\right] \ . \tag{9}$$

With the use of Eqs. (5), (6), and (8) we get the self-consistent equations[4]

$$\omega = Na_0^* u(\omega) + \frac{1}{\pi}\int \frac{V^2(q)[u(\omega)-V(q)]}{[u(\omega)-V(q)]^2+s^2(\omega)}dq \tag{10}$$

and

$$Na_0^* = \frac{1}{\pi}\int \frac{V^2(q)}{[u(\omega)-V(q)]^2+s^2(\omega)}dq \ , \tag{11}$$

where $q = ka_0^*$ and $V(q) = a_0^* V(q/a_0^*)$.

For 1D lattices, $\mathrm{Im}[G_{ii}(\omega)]$ shows discontinuities at $\omega = E_1$ and $\omega = E_u$, where $E_1$ and $E_u$ are the lower and upper band edges, respectively, given then the impurity bandwidth. The $\mathrm{Re}[G_{ii}(\omega)]$ diverges at $E_1$ and $E_u$. The $u(\omega)$ and $s(\omega)$ are obtained self-consistently from Eqs. (10) and (11).

In GaAs where the electron effective mass is $m^* = 0.067m_0$ and the dieletric constant $\kappa = 13$, the effective Rydberg unit is $R^* = 5.3$ meV and the Bohr radius is $a_0^* = 100$ Å. We will adopt these units. The variational solution for the isolated impurity is given by

$$E = \langle \Psi | -\nabla_{xyz}^2 - \frac{2}{r} + V(x,y) | \Psi \rangle \ , \tag{12}$$

where $V(x,y) = \infty$ outside and zero inside the wire of dimension $L$. We use the function[12]

$$\Psi(r) = N_\lambda \left[\frac{2\lambda}{\pi}\right]^{1/4} \cos(\pi x/L)\cos(\pi y/L) \times \exp[-\lambda(x^2+y^2+z^2)] \tag{13}$$

with $|x|, |y| \le L/2$, and zero otherwise and $\lambda$ a variational parameter. $N_\lambda = 2\int_0^{L/2}\cos^2(\pi x/L)\exp(-2\lambda x^2)dx$ is the normalization constant. The impurities are located at the center of the quantum wire. Considering the impurities distributed around the center of the wire, the values of the energies will present a small variation. We take a constant value for the energies which reduces the problem to the treatment of only the off-diagonal $V_{ij}$ matrix elements.[14] After obtaining $\lambda$ numerically by minimizing $E$, for each $L$, we calculate the following expressions: the binding energy $E_B$

$$E_B = 2\left[\frac{\pi}{L}\right]^2 - E \tag{14}$$

and the hopping energy $\langle i | e^2/K(|\mathbf{R}_i - \mathbf{R}_j|) | j \rangle$, i.e.,

$$V(R,L) = \left[E_c - 2\lambda R\left[\frac{2\lambda}{\pi}\right]^{1/2} + (\lambda R)^2\right] S(R,L) \ , \tag{15}$$

where $E_C$ is the Coulomb energy, $|\mathbf{R}| = |\mathbf{R}_i - \mathbf{R}_j|$, and $S(R,L)$ is the overlap integral $\langle i | j \rangle$, i.e.,

$$S(R,L) = \exp(-\lambda R^2/2) \ . \tag{16}$$

In Fig. 1 we show the peak energy $E_P(L)$ obtained at the maximum of $D(E)$, i.e., $D(E_P)$, and the bandwidth

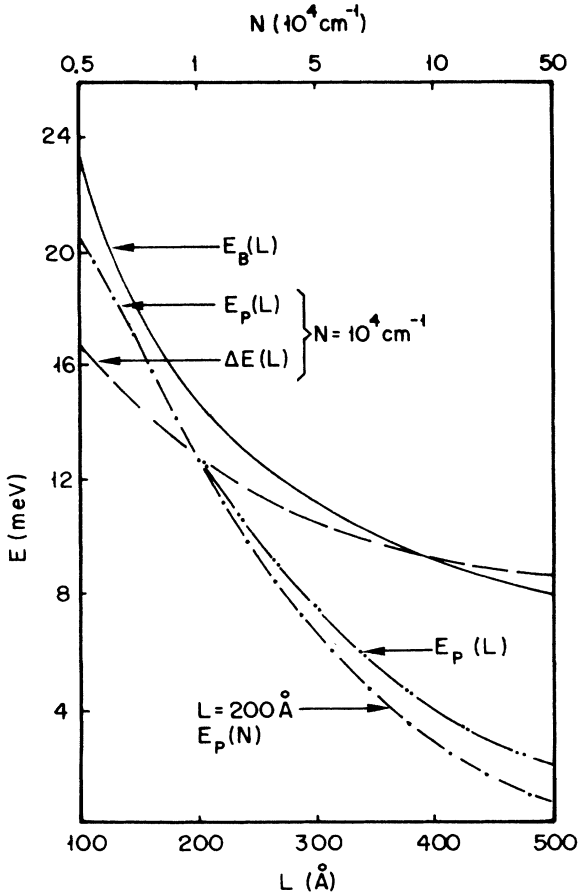

FIG. 1. Variation of binding energy $E_B(L)$, peak energy $E_P(L)$ of maximum $D(E)$, and bandwidth $\Delta E(L)$ with the wire dimension L. Upper scale represents $E_P(N)$ for $L = 200$ Å, as a function of impurity concentration $N$.

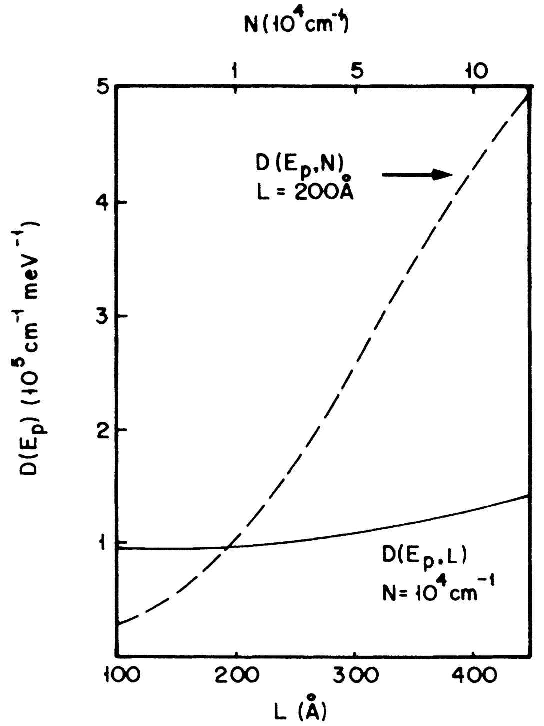

FIG. 2. Maximum of the impurity density of states $D(E_P)$ as a function of $L$ and $N$. Upper scale represents $D(E_P,N)$ for $L = 200$ Å as a function of $N$. Lower scale refers to $D(E_P,L)$ for $N = 10^4$ cm$^{-1}$ as a function of $L$.

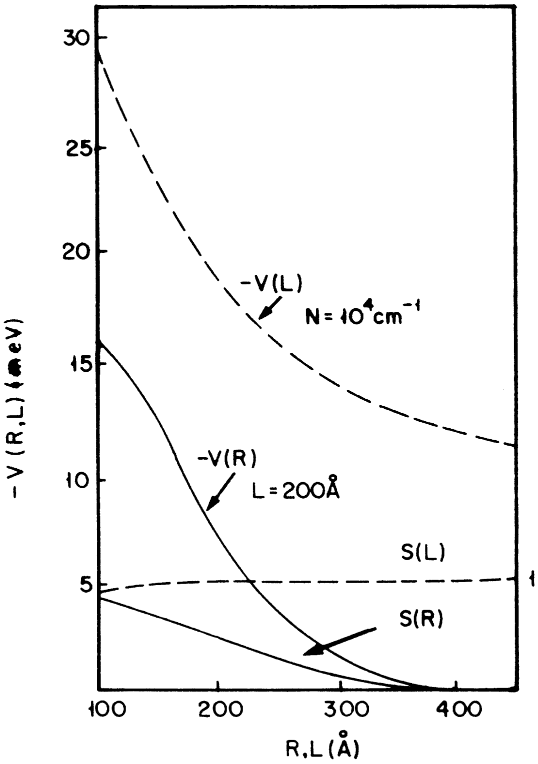

FIG. 3. Hopping energy $V$ and overlap integral $S$ vs interimpurity distance $R$ and $L$. Right scale represents $S(R,L)$.

$\Delta E(L)$ for $N=10^4$ cm$^{-1}$, $E_B(L)$, and $E_P(N)$ for $L=200$ Å. It is worth pointing out that $E_B \rightarrow 5.3$ meV for a large value of $L$ ($L \gg a_0^*$). It corresponds to $E_B$ of a donor in GaAs. For $L \rightarrow 0$ the electron wave function will recover $Ga_{1-x}Al_xAs$. For the sake of comparison $L=100$ Å corresponds to $E_B=24$ meV, a similar value found by Brum.[15] Lee and Spector[16] found 17 meV and Bryant,[17] for a cylindrical cross section, found 16 meV. It is noticed also that for $L=200$ Å the system undergoes a similar energy around 13 meV for all calculated properties. This brings our attention to the observed cathodoluminescence in the GaAs-$Ga_{1-x}As_xAl$ heterojunction with $L=200$ Å, by Petroff *et al.*[10] They observed a broader linewidth of 15 meV, with a full width at half maximum. We have obtained from it 12 meV. The peak energies $E_P(L)$ and $E_P(N)$ decrease with a small difference between them. For some approaches which use the center of gravity $E_{CG}(L)$ instead, as function of $L$, and have impurity bands with many structures,[9] one can expect $E_{CG}(N)$ to have the same behavior as $E_{CG}(L)$.

In Fig. 2 we show the behavior of $D(E_P,N)$, for $L=200$ Å and $D(E_P,L)$ for a known $N$ (here we use $N=10^4$ cm$^{-1}$, a linear density for the mean interimpurity distance along the $z$ axis). The crossing of the curves gives $D(E_P)$ around $10^5$ cm$^{-1}$meV$^{-1}$. It corresponds to $L=200$ Å and $N=10^4$ cm$^{-1}$.

In Fig. 3 we show the hopping energy and overlap. The hopping energy has a remarkable enhancement for smaller $L$ or $R$. This will give a broader bandwidth. For $L>100$ Å it will have the same value of $E_C$. For $L=200$ Å $V(R)$ will decrease rapidly for large $R$ given a smaller bandwidth. On the other hand for fixed $N$, $V(L)$ and $S(L)$ will play a different role in the formation of the impurity band. $V(L)$ will decrease smoothly and $S(L)$ will increase up to its maximum value. These combined effects, for such doping concentration, will always give a reasonable impurity band.

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