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Proposal for neutral donors in quantum wells to act as charge storage centres for room temperature single electron memories

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Abstract. This work discusses a range of semiconductor materials, and demonstrates that in a II–VI compound semiconductor, the neutral donor binding energy can be enhanced with the addition of a quantum well confining potential, to a value greater than kT at room temperature and simultaneously greater than the longitudinal optic phonon energy. Thus room temperature occupation is a possibility. The application of this nanoscale localisation centre as a single electron memory is discussed.

1 Introduction

This work is motivated by the question: *‘What is the smallest centre of localisation that can be used to store a single bit of information?’* One possibility is a single impurity atom within a host semiconductor. For example, an unoccupied (ionised) donor atom could represent a ‘0’ and an occupied (neutral) donor could represent a ‘1’. The fundamental physics that would have to be satisfied to make such a system interesting would be to have control over the occupational state of the donor at room temperature. This relies on two points: *‘Can the electron bound to the donor be resistant to ionisation and how can one read/write the information within a device?’* In the sections below I will show theoretically that shallow hydrogenic donors can be engineered to resist ionisation by phonons at room temperature and thus exhibit long storage lifetimes. Then the work will move on to consider incorporation into contemporary single electron device geometries and possible optical read/write techniques using far-infrared lasers currently under development.

Table 1. LO phonon energies in selected bulk compound semiconductors (LTO mode for Si)

Material	Phonon energy (meV)	Material	Phonon energy (meV)
Si	62	InAs	30
AlAs	50	ZnS	43
GaP	50	ZnSe	31
InP	43	ZnTe	26
GaAs	36	CdTe	21

Simplistically one might think that the first point can be satisfied by choosing a donor and host material with a binding energy E_b larger than kT at room temperature (25 meV). In fact the criteria is more stringent than this in that the binding energy must be large enough to resist ionisation by common large energy (usually longitudinal optic (LO)) phonons. Table 1 gives examples of phonon energies in a selection of group IV,

III–V and II–VI. It is clear that the LO phonon energy E_{LO} is generally smaller in II–VI materials and in fact satisfying the criteria of $E_b > kT$ in CdTe will also satisfy $E_b > E_{LO}$. The neutral donor binding energy in bulk CdTe is less than E_{LO} , however it can easily be enhanced by placing the donors in a quantum well [1]. Furthermore very high quality CdTe–Cd_{1–x}Mn_xTe quantum well structures can be grown, with photoluminescence linewidths less than 1 meV [2].

2 Theoretical methods

The centres of localisation (or storage) of electrons are proposed to be donor atoms in quantum wells. As stated above the quantum well potential is to be utilized in order to increase the binding energy of the neutral donor with the aim of storing the charge at room temperature and resisting ionisation by phonons. Therefore an accurate evaluation of the neutral donor binding energy within a quantum well needs to be made. The original variational approach of Hagston *et al.* [1] is employed. The trial wave function is chosen as

$$\Psi = \chi(z) \exp\left(-\frac{r''}{\lambda}\right), \quad r'' = \sqrt{x^2 + y^2 + \zeta^2(z - r_d)^2} \quad (1)$$

where the envelope $\chi(z)$ is determined by forming the time independent Schrödinger equation integrating over the in-plane $(x - y)$ co-ordinates and solving the resulting differential equation using a numerical shooting technique [1].

Recently Roberts *et al.* [3] have shown that the lowest energy solutions, and therefore the most accurate, are indeed obtained by allowing ζ to vary the symmetry of the trial wave function Ψ . However good approximations are also obtained by setting $\zeta = 1$, i.e. a spherically symmetric relative motion term, with differences less than 0.1 meV. This approximation will be made in this work in the interests of reducing the, otherwise, considerable computational effort.

The envelope function approximation on which these theoretical methods are based, depends crucially on the quality of the parameterization of the material parameters, in particular the band offset, the electron effective mass, and the dielectric constant. The first, the band offset, has been deduced through carefully comparison with theory and experiment to be around 30% [2]. Hence the conduction band offset as a function of the manganese concentration in the barrier is $0.7 \times 1587x$ meV. Note that as the effective mass is related to the band structure, which itself is a function of the carrier momentum $\mathbf{k}$, then the effective mass is also a function of $\mathbf{k}$. In its simplest form this manifests itself as ‘non-parabolicity’ often referred to in calculations of one-dimensional systems, see Long *et al.* [4] and references therein. However in a two-dimensional system such as this, the $\mathbf{k}$ -space sampling of the bound electron arises from the real-space circular orbit. Harrison *et al.* [5] calculated the electron effective mass for the same material system as this but for an electron bound to a heavy-hole in an exciton. This effective mass of $0.11m_0$ is employed in this similar system. In addition the work of Harrison *et al.* also deduced the relevant dielectric constant $\epsilon \approx 9$, which is between the static (10.6) and high frequency (7.4) values, by careful comparison of detailed theoretical calculations with experimental measurements. It should be noted that the main conclusions of this work are not dependent upon the specific values chosen for these material parameters.

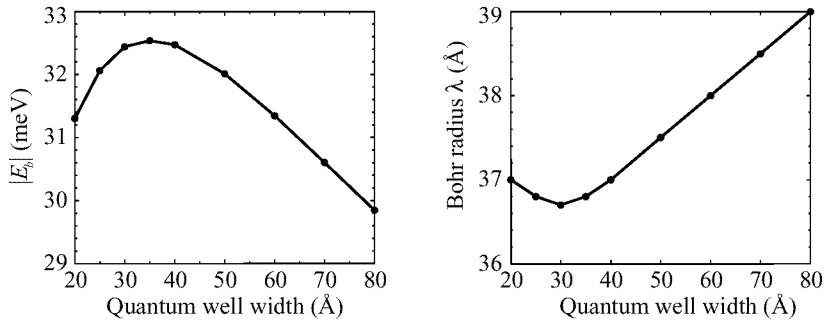


Fig 1. (a) Neutral donor binding energy and (b) Bohr radius, for donors at the centre of a well, as a function of well width.

3 Results and discussion

3.1 Maximising the neutral donor binding energy

For any given material system the neutral donor binding energy within a quantum well is a function of three variables, the donor position, the quantum well width and the quantum barrier height. Earlier work [1, 3] has already established that the neutral donor binding energy is a maximum when the donor is located at the centre of the well. Hence only the second and third degrees of freedom need be explored in order to maximise the binding energy. Figure 1(a) displays the magnitude of the binding energy as a function of well width, it is clear that it displays a peak of 32.5 meV at a well width of 35 Å. This value is larger than kT at room temperature, though more importantly it is considerably larger than the bulk LO phonon energy of 21 meV, hence it will be resistant to ionisation by phonon scattering. Assuming a simple Bohr atomic model would imply that the first excited state of the donor is $1/4$ of the ground state binding energy, i.e. around 8 meV, further implying that the energy for excitation is $32.5 - 8 \approx 24$ meV. Which means that LO phonons could not excite the occupied donor at all, which is a very important point as an excited donor could be ionised by a second phonon. Fig. 1(b) displays the corresponding Bohr radii λ . It gives an indication of the size of the donor ‘quantum dot’. The maxima in binding energy corresponds closely with the minima in this localisation radius, which would determine the packing density.

Additional calculations have shown that the binding energy can be enhanced further by up to 2 meV with increasing manganese content in the barriers. Though it is acknowledged that the material quality tends to decrease for higher alloy concentrations.

3.2 Incorporation of single donor ‘dot’ into a device

There are several ways in which the donor ‘quantum dot’ could be incorporated into existing single electron devices. For example, it could be used to replace the quantum dot ‘floating gate’ used in single electron MOS memory, recently demonstrated at room temperature [6]. In this device charge stored on a floating gate, which is varied by a control gate, affects the threshold voltage of a transistor, thus allowing the information to be read. Similarly a ‘donor dot’ whose occupancy is controlled by a side gate could be utilized as a source for the ‘Coulomb blockade’ of single electron transport from a source to a drain.

Perhaps more long term, the donors could be the building block of an optical read/write memory system. Information could be written on a fully occupied δ -layer by selective ionisation with a laser tuned to the donor binding energy, with the ionised carriers swept away by a static electric field. The information is then represented by the occupancy state of single (or perhaps groups of) donors. It could be read by a lower energy laser tuned to the excitation from the ground state to the first excited state. Light falling on a region of ionised donors would be transmitted, regions of occupied donors would be temporarily excited and disperse the radiation. Research into the required terahertz lasers is underway.

4 Conclusion

In summary it has been demonstrated that the neutral donor binding energy can be enhanced with a quantum well to a level where ionisation can be resisted at room temperature. The possible application as a room temperature single electron memory has been discussed.

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