OPTICAL PROPERTIES OF SHALLOW DONOR NEAR SEMICONDUCTOR-METAL INTERFACE

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Intraband transitions of an impurity electron from the ground state to $2P_x$ and $2P_y$ excited states of a shallow donor located near a semiconductor-metal interface are investigated as a function of the donor distance from the interface. Impurity states are calculated within the effective mass approximation and using a variational scheme in which the energies and the oscillator strength for the intraband absorption are obtained analytically.

Keywords: Interface; metallic gate; shallow donor; intraband absorption

1. Introduction

Dopant atoms in semiconductors and its heterostructures create essential changes in electronic and optical properties. On the other hand, today dopant atoms could be used as the functional part of a device instead of just providing charges. An example is the proposal of Kane¹ to use donor states as qubits.

The investigation of the energetics and optical properties of dopant atoms in nanoscale devices and near different interfaces is a very important topic of research in recent years from theoretical as well as from experimental point of view to anticipate future applications in opto- and nanoelectronics.

In Ref.2 electron energy loss spectroscopy was combining with annular dark-field scanning transmission electron microscopy (ADF-STEM) to image individual Mn impurities inside ZnSe nanocrystals

Due to further miniaturization of semiconductor devices the dopant atoms appear closer and closer to interfaces and correspondingly the study of such impurity states by different methods becomes a problem of fundamental interest. A direct and flexible technique to investigate dopant atoms close to the surface is proposed by the method of scanning tunneling microscopy (STM). The electrostatic potential induced by the STM tip allows manipulating the charge state of individual impurities near the surface of the semiconductor^{3,4}.

As it is well known, the engineering of the electronic structure of materials is possible by means of shape and size control of semiconductor nanostructures. Today the tailoring of

the energy spectrum of shallow dopant atoms is possible in alternative way, using different positions of dopant atoms near various interfaces (semiconductor-metal or semiconductor- dielectric) to produce desirable intra- and inter-band optical transitions. The investigation of these optical transitions can be useful for the development of optoelectronic devices with tunable emission or transmission properties and ultra-narrow spectral line widths.

The absorption spectra in the infrared energy range in distinct triple GaAs-(Ga, Al)As quantum-well heterostructures connected with intra-donor transitions in external electric and magnetic fields is investigated in Ref. 5.

The influence of different factors, such as the confinement geometry, valley degeneracy, crystallographic orientations, and anisotropy of the effective mass on the intraband absorption of Si nanocrystals is theoretically studied in Ref.6.

In Ref.7 shallow donor far infrared spectroscopy was experimentally carried out on n-type CdTe thin layer doped by indium. The layers were grown on an undoped CdTe buffer whose thickness d_b varied from sample to sample. It was shown experimentally in Ref.7 that the shape of the spectra for the $1s-2p+$ intra-donor transition changes with d_b . These changes are related to the degree of structural disorder that originates from the GaAs/CdTe interface and fades out with the increased distance from the interface.

In our previous work ⁸ we investigated the lowest electronic states of a donor located near a semiconductor-insulator-metal plane interface within the effective mass approximation using a variational approach, which takes into account the influence of all image charges that arise due to the presence of the metallic and the dielectric interfaces. The results for semiconductor-metal interface were compared with a numerical exact calculation using the finite element technique ⁹ and a good agreement was obtained.

For the fundamental physics as well as for the applications it is interesting to develop analytical methods for the solving such problems with a few charged particles interacting via Coulomb potential.

Such analytical results for wavefunctions and the energies for an impurity electron near an interface can be useful also for the investigation of optical properties of these systems.

In this work we theoretically study the intraband light absorption between lowest energy states of a shallow donor near semiconductor-metal interface. We use a variational approach in which the energies $1S$, $2P_x$, $2P_y$ and the oscillator strength for the intraband absorption $1S \rightarrow 2P_x$ and $1S \rightarrow 2P_y$ are obtained analytically as a function of the donor distance from the interface. We hope that such investigation will be useful for the creation of new optoelectronic devices operating within this energy transition range.

The present paper is organized as follows. Section 2 contains an outline of the theory and gives closed analytical expressions for the trial wave functions of the ground and excited $2P_x$ and $2P_y$ states. Section 3 presents the theory for intraband absorption and Section 4 presents the results together with the main conclusions.

2. Impurity near a semiconductor-metal interface with a thin dielectric layer

For the case of the semiconductor-metal interface case is assumed, that the oxide layer between semiconductor and metal is very thin and creates only an infinitely high potential barrier, which prevents the electron penetration into the metal. Due to its thickness the oxide layer does not contribute to the dielectric mismatch.⁸ On the contrary, the metallic gate screens Coulomb potential. The permittivity at the semiconductor side of the interface $\epsilon_1 = 11.9$, while it is infinite in the metal. The dielectric mismatch effects at the interface give rise to image charges that screen the potential between the electron and the impurity. The potential between an electron and an impurity near the semiconductor/metal interface on the distance d has a form

$$W = \frac{e^2}{4\pi\epsilon_1} \left[-\frac{1}{4z} + \frac{1}{\sqrt{\rho^2 + (z+d)^2}} - \frac{1}{\sqrt{\rho^2 + (z-d)^2}} \right], \quad \rho = \sqrt{x^2 + y^2}. \quad (1)$$

The first term describes the attractive interaction between the electron and its image, the second term is due to the repulsive interaction between the electron and donor image (as well as between the donor and the electron image) and the last term represents the normal impurity-electron interaction.

The profile of the impurity electron potential along the z -axis (with $\rho = 0$) for semiconductor/insulator/metal case with infinitely thin dielectric layer⁹ exhibits a double well structure. When the impurity moves toward the interface, the potential wells start to interact strongly and eventually combines into a single well.

Fig.1 (Color online) Potential energy of the impurity electron near semiconductor-metal interface along the z axis ($\rho_e = 0$) for two different impurity positions.

In the cylindrical coordinates, in dimensionless units of Bohr radius $a_B = \hbar^2 \epsilon_1 / m_{\perp} e^2$ and twice Rydberg energy $2R^* = \hbar^2 / m_{\perp} a_B^2$, the Hamiltonian of the system is

$$H = -\frac{1}{2} \left[\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{m}{\rho^2} + \gamma \frac{\partial^2}{\partial z^2} \right] + \left(-\frac{1}{4z} + \frac{1}{\sqrt{\rho^2 + (z+d)^2}} - \frac{1}{\sqrt{\rho^2 + (z-d)^2}} \right), \quad (2)$$

where γ is the ratio between the transverse and longitudinal effective masses. We have chosen the ground state variational wave function ψ of the system in a form ⁸:

$$\psi_0 = N z \exp(-\lambda \sqrt{r^2 + (z-d)^2}) \exp(-\beta z); \quad (3)$$

due to the factor z the wave function satisfies the boundary condition $\psi(z=d)=0$; λ, β are the variational parameters. The exponential factor $\exp(-\beta_1 z)$ describes the influence of the electron with the images.

For $(2, 1, +1)$ and $(2, 1, -1)$ states we choose the following variational functions ^{10, 11}.

$$\psi_{2p_x} = N \exp(-\lambda_{2p_x} r) \rho \cos \varphi f(z); \quad (4)$$

$$\psi_{2p_y} = N \exp(-\lambda_{2p_y} r) \rho \sin \varphi f(z). \quad (5)$$

3. Oscillator strength

The optical absorption calculation of shallow donor is based on the Fermi's golden rule. The intraband absorption coefficient, in electric dipole approximation, is given by the expression

$$w = \frac{4\pi^2 e^2}{\epsilon \hbar^2 c} I(\omega_{kn}) \left| (\mathbf{er})_{l,u} \right|^2, \quad (6)$$

where $I(\omega_{kn})$ is the intensity of the electromagnetic field at the frequency $\omega_{l,u} = (E_l - E_u) \hbar^{-1}$, where E_l and E_u are the energies of initial and final states correspondingly (the subscripts l, u indicate the lower (initial) and upper (final) transition states); $(\mathbf{er})_{l,u}$ is the electric dipole matrix element for the transition from the state l to u and is given by

$$(\mathbf{er})_{l,u} = \langle \psi_u | \mathbf{er} | \psi_l \rangle = f_{ul}, \quad (7)$$

where ψ_u and ψ_l are normalized wave functions of the final and initial states correspondingly.

The study of optical transitions in terms of the dimensionless oscillator strength F_{ul} is also convenient and gives information on the structure and selection rules of the optical absorption. The quantity of F_{ul} is defined by

$$F_{ul} = \frac{2m(E_u - E_l)}{\hbar^2} \left| \langle \psi_u | \mathbf{e} \mathbf{r} | \psi_l \rangle \right|^2 = \frac{2m(E_u - E_l)}{\hbar^2} f_{ul}^2 \quad (8)$$

We consider the absorption by shallow donor of circular polarized light (with two possible circular polarization of photons), when the polarization vector $\mathbf{e}$ is in the XY plane. The selection rule in this case is $m_u = m_l \pm 1$.

For projections $\mathbf{e}_x$ and $\mathbf{e}_y$ of polarization vector $\mathbf{e}$ we have¹²

$$(\mathbf{e}_x + i\mathbf{e}_y) \mathbf{r} = x + iy = -r \sqrt{\frac{8\pi}{3}} Y_{1,1}; \quad (\mathbf{e}_x - i\mathbf{e}_y) \mathbf{r} = x - iy = r \sqrt{\frac{8\pi}{3}} Y_{1,-1} \quad (9)$$

Using the expressions for wave functions given by Eqs. (3) – (5) and Eq. (9), for the matrix dipole element of shallow donor intraband transition $1S \rightarrow 2P_x$, after integration over φ in Eq. (8), we finally obtain

$$f_{1S \rightarrow 2P_x}(d) = \frac{2\pi \int_0^\infty \int_0^\infty z^2 \exp(-\beta_{1s}z) \exp(-\beta_{1s}z) \exp(-\lambda_{1s}r) \exp(-\lambda_{2p}r) \rho^3 d\rho dz}{\sqrt{A_1(\lambda_{1s}, \beta_{1s}) A_2(\lambda_{2p}, \beta_{2p})}} \quad (10)$$

where $\lambda_{1s}, \lambda_{2p}, \beta_{1s}, \beta_{2p}$ are the optimal values of variational parameters for $1S$ and $2P$ states obtained for fixed value of d ;

$$A_1(\lambda_{1s}, \beta_{1s}) = 2\pi \int_0^\infty \int_0^\infty z^2 \exp(-2\beta_{1s}z) \exp(-2\lambda_{1s}r) \rho d\rho dz, \quad (11)$$

$$A_2(\lambda_{2p}, \beta_{2p}) = 2\pi \int_0^\infty \int_0^\infty z^2 \exp(-2\beta_{2p}z) \exp(-2\lambda_{2p}r) \rho^3 d\rho dz \quad (12)$$

The same expression is valid for the transition $1S \rightarrow 2P_y$, so the matrix elements for these transitions are equal.

4. Discussion

The results obtained for the ground and excited states energies are presented in Fig.2 for the case of equality of the transverse and longitudinal effective masses. The energies of $2P_x$ and $2P_y$ states are equal to each other; this degeneracy can be lifted, e.g. by

external magnetic field. In the region of close distances of the donor from the interface ($d \sim a_B$), the account of factor $f(z) = \exp(-\beta z)$ is very important, and gives for small distances of the donor from the interface the energy lowering more than 10%. We have compared our results with “exact consideration” based on finite element method, and obtained a good agreement: the relative mistake is less than 2% when the impurity distance $d \geq 2a_B$ from the interface. For smaller distances, when $d = a_B$, the relative mistake is less than 10 %. For $d = a_B$ the electron charge distribution is strongly non spherical.

Fig.2 (Colore online) The dependence of shallow donor 1S and $2P_x$ states (in units of $2R^*$) as a function of the donor position d/a_B (with respect to the metal interface) for the semiconductor/metal interface problem. For the comparison energies of the system in the absence of the image effects are also presented.

As is shown in Fig.2, the energetic interval between 1S and 2P states, in the region of small d , essentially depends on the donor distance from the interface. The account of image charges leads to the decrease of the energies.

On the basis of energies obtained, the intraband transitions from the ground state to $2P_x$ ($2P_y$) excited states of the electron of shallow donor located near a semiconductor-metal interface are investigated as a function of the donor location from the interface.

Fig.3 shows the results obtained for electric dipole matrix element calculated for $1S \rightarrow 2P_x$ intraband transition of shallow donor near semiconductor metal interface in the case of circular photon polarization in the plane of the interface (XOY). Solid line in Fig.3 shows the results obtained, when we take into account all image charges arising due to the presence of metallic gate. The dot-dashed line presents the results obtained for f_{ul} , when we ignore the image charges.

Fig.3 (Colore online) The dependence of electric dipole matrix element $f_{ul} = \left| \langle \psi_u | \mathbf{er} | \psi_l \rangle \right|$ for the intraband $1S \rightarrow 2P_x$ transition of shallow donor located near a semiconductor-metal interface as a function of the donor distance from the interface taking into account the influence of charge images solid line (solid line) and without charge images (dot-dashed line).

As it is expected, the oscillator strength is a monotonically increasing function of the distance d of the donor from the interface. The transition probabilities are small near the interface because of small overlapping of the wave functions of the ground and excited states. When the donor is localized at the distance d about of effective Bohr radius, the electronic wave functions are spread out along the interface.

We observe a rapid increase of f_{ul} in the region of small values of d , where f_{ul} is small. For large values of the donor distance from the interface and when we ignore the image charges, the oscillator strength as well as the ground and excited state energies tend to the bulk limit (see Fig.2 and Fig.3.).

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