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PHYSICAL PROPERTIES OF DONOR STATES NEAR THE SEMICONDUCTOR SURFACE IN AN EXTERNAL ELECTRIC FIELD

The ground state energy and the extent of the wave function of a neutral donor located near the semiconductor surface in the presence of an electric field created by the Scanning Tunneling Microscope metallic tip (or a metallic sphere) is obtained within a variational approach that takes into account the influence of all image charges. The ionization process of a donor center due to the tip positive voltage is considered. A possibility of applying the results obtained to create a new type of gas detector (sensor) is discussed.

Keywords: donor states, image charges, interface, scanning tunneling microscope tip.

1. INTRODUCTION. The enhanced interest in studying the shallow donor impurities near an interface (either with vacuum or in metal-oxide-semiconductor interfaces) is related with its very promising application in the atomic scale electronics, quantum computing and nanoelectronics. An example is the proposal of Kane to use donor states as qubits [1]. Due to the increased miniaturization, the oxide layer (between the semiconductor and the metallic gate) is strongly reduced in thickness and the screening effect of the metallic gate becomes very important. This motivated us to develop a variational approach for shallow donor states localized in a semiconductor at a semiconductor-insulator-metal interface in the absence of [2] as well as in the presence of [3] of a magnetic field, taking into account the image charges i.e. solving such problems with a few charged particles interacting via the Coulomb potential. A direct and flexible experimental 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 tip allows manipulating the charge state of individual impurities near the surface of the semiconductor [4, 5]. The manipulation is fully controlled by the position of the tip and the voltage applied between the tip and the sample.

It is very interesting to theoretically investigate the effect of the electric field created by a metallic sphere, and also of the electric field created by STM tip, on the donor states located near the interface. We used the s-wave-tip model of the STM tip suggested in Ref.6 and Ref.7, where a probe tip can be of an arbitrary shape but is assumed locally spherical when it approaches the semiconductor surface. We investigated theoretically the effect of **neutral STM metallic tip** on the donor binding energy and the electron wavefunction when a neutral donor is placed near a semiconductor-vacuum surface [8]. In this paper, the binding energy of the shallow donor located near a semiconductor surface in the presence of STM tip held at a fixed potential is investigated.

2.THEORY

2.1. The configuration of the system

We consider the ground state energy of a neutral donor located near the surface of a semiconductor in the presence of a charged STM tip, which we approximate by a metallic charged sphere. We assume that the vacuum layer between the tip (sphere) and the semiconductor surface ($XO'Y$ plane) near point O′ in Fig.1 is very thin and does not contribute to any dielectric mismatch and thus only the metallic tip screens the Coulomb potential. The value of the static dielectric constant ε for typical semiconductors of interest is about 10 while we take it infinity in the metal. Our numerical calculations are done for Si doped *GaAs* with the effective Bohr radius $a_B^* = \hbar^2\varepsilon / m_e e^2 \simeq 100A^0$ and the effective Rydberg energy $R^* = e^2 / 2\varepsilon a_B^*$ =5.15meV, where m_e is the effective mass. The potential created by the impurity electron in the tip vicinity can be found using the method of images.

2.2. The vertical position of the tip

Here we consider the case when the tip is positioned just above the donor which is located at the point *D* (see Fig. 1a) on the z-axis (i.e. the center of the tip is on the z-axis) and approaches the semiconductor only in the z-direction.

The potential energy of the impurity electron (with the charge −*e*) at point *A* near the donor impurity (with charge *q* = *e*) located at point *D* (at the distance $d = O'D$ from the semiconductor surface) in the presence of the STM tip (the sphere with the radius *a*) held at a fixed potential is:

$$U_{Coul} = e^2/\varepsilon\left[-a/2OA\cdot CA + a/OD\cdot AB - 1/AD - n/OA\right], \qquad (1)$$

where $e' = ea / OA$ is the electron image which arises at point *C* at the distance $OC = a^2 / OA$ from the tip center; the donor image $q' = -ea / OD$ is located at point *B* at the distance $OB = a^2 / OD$ from the center of the tip. The first term in Eq.(1) describes the attractive interaction between the electron and its image, the second term is due to the repulsive interaction between the electron and the donor image, as well as between the donor and the electron image, and the third term represents the normal impurity-electron interaction.

The term n / OA in Eq. (1) describes the STM tip electric field effect, i.e. the interaction of the electron with the charge $ne(n = \pm 1, 2..)$ and *OA* is the distance of the electron from the sphere center. Since the problem is cylindrically symmetric, we use cylindrical coordinates with the center in point *O′* with the z-direction through point *D*. We find the following expressions for the distances: the distance *CA* between the electron and its image is

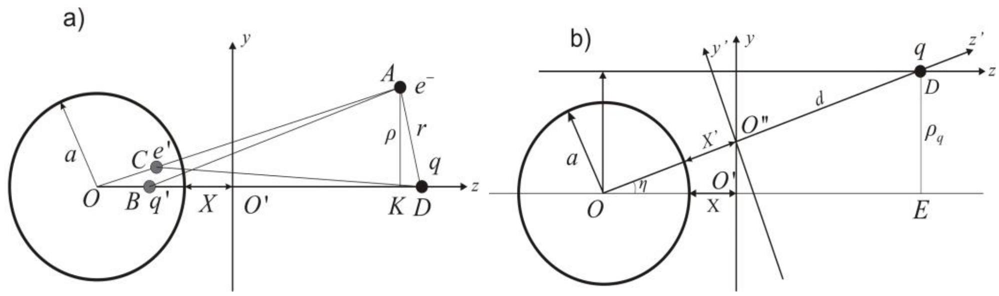

Fig. 1. Schematic picture of the system configuration in the case when the tip: (a) is placed on top of the donor; (b) is shifted (non-central) laterally with respect to the donor. The donor is positioned at point D

$$CA = \frac{\rho^2 + (a' + z)^2 - a^2}{OA},\ OA = \sqrt{\rho^2 + (a' + z)^2}; \tag{2}$$

the distance *BA* between the electron and the donor image is

$$BA = \sqrt{\rho^2 + \left(z + X + \left(a - \frac{a^2}{a' + d}\right)\right)^2}\ , \tag{3}$$

the distance *AD* of the electron from the impurity is $AD = \sqrt{\rho^2 + (z-d)^2}$ and the donor-tip center distance is $OD = a + X + d = a' + d$ with *X* being the interval between the tip and the semiconductor surface.

In dimensionless units expressed in terms of the effective Bohr radius and twice the effective Rydberg energy, the Hamiltonian of the system is

$$H = -\frac{1}{2}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{m}{\rho^2} + \frac{\partial^2}{\partial z^2}\right] + U_{\text{Coul}}(r)\,. \tag{4}$$

We choose the ground state variational wave function of the system as

$$\psi = Nz\exp(-\beta CA)\exp(-\lambda r), \tag{5}$$

where $r = AD = \sqrt{\rho^2 + (z-d)^2}$. This wave function satisfies the boundary condition $\psi(z=0) = 0$ where β and λ are variational parameters. The ground state energy of the system is given by

$$E = \frac{\iint \psi^* H \psi \rho d\rho dz}{\iint |\psi|^2 \rho d\rho dz}\ . \tag{6}$$

3. The negatively charged tip. The application of a positive sample voltage on the STM tip causes a depletion area under the tip near the semiconductor surface, which decays into the bulk. At some critical voltage, the electron is repelled from the donor center and released into the conduction band [4, 5]. In the present work, to obtain the parameters (a, X, n) for ionization of the donor placed at a depth d, we minimize the energy of the system given by Eq. (6). In the case of a charged tip with positive voltage (positive potential energy for impurity electron) we assume that there is one negative elementary charge on the tip $n = -1$ which creates the potential $V = -e / \varepsilon a$ on the tip. For different values of the parameters a and d, we find the critical distance between the tip and the semiconductor surface X_c, at which the total energy of the system is near zero, i.e. the system is close to the ionization.

We plotted in Fig. 2a the dependence $X_c(d)$ for two different values of the tip radii ($a = 0.5a_B^*$ and $a = 0.2a_B^*$) for which the energy is 10^{-3} in units of $2R^*$, i.e. 10^{-2} meV. The corresponding dependencies for the average positions $< z - d >$ and $< \rho >$ are shown in Fig. 2b.

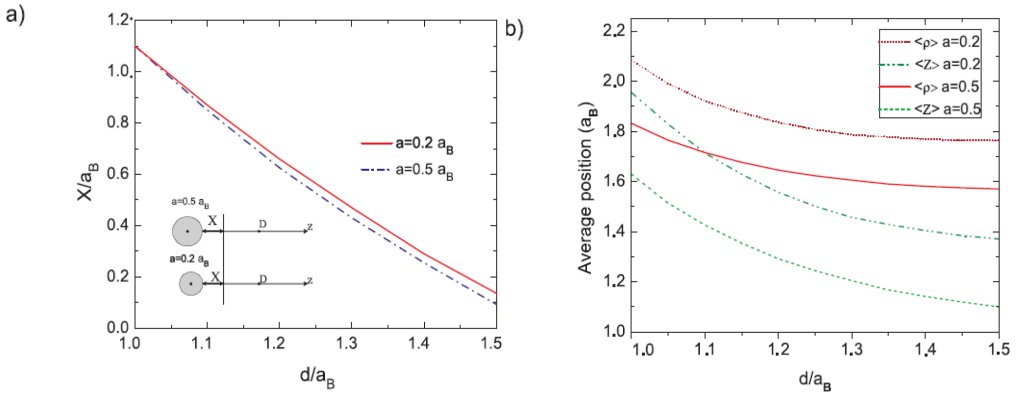

Fig. 2: a) The dependence of the critical value of the tip-semiconductor distance X for donor ionization (for two different values of the tip radii $a = 0.5a_B^*$ and $a = 0.2a_B^*$) on the distance d when the charge of the tip is −e (i.e. $n = -1$). Inset: schematic representation of the studied systems; b) The corresponding average positions of the electron $< \rho >$ and $< z - d >$ as a function of d for $a = 0.5a_B^*$ and $a = 0.2a_B^*$ when the donor is almost ionized; the energy is about $10^{-3}(2R^*)$

It is clear that for the fixed distance X, the effect of the tip voltage is stronger for a smaller tip. Indeed, with increasing the tip size this effect becomes weaker since the center of a larger tip is farther from the donor, while the effect of the images becomes stronger.

As a consequence, when we change the tip radius from $a = 0.2a_B$ to $a = 0.5a_B$ the influence of the tip charge decreases (leading to a tiny decrease in the tip term in the potential of about $0.04R^*$), meanwhile the role of the image charges increases (leading to a small positive shift in the first term which compensates this decrease in the tip term) and so the total shift remains the same and leads to a zero total energy. As a result, as shown in Fig. 2a, for both values of the tip radius $a = 0.5a_B$ and $a = 0.2a_B$ at the donor depth d = 1, the critical distance X_c equals $X_c = 1.1$.

From mathematical point of view, the solved problem is identical to another one, namely, when a **metallic sphere** with radius a is placed near a semiconductor surface.

It should be noted that our calculations are performed for any radius of the metallic sphere and not only for small sizes connected with the tip radius. The results obtained show that the donor binding energy ***is very sensitive*** to the tip voltage or to the voltage applied to ***a small metallic sphere*** located near the semiconductor interface. This fact gives us the possibility to apply the results for developing new methods for gas sensor creating.

The negative charge on the metallic sphere can be formed e.g. by the absorption of oxygen ions from the atmosphere which leads to the formation of the depletion layer and to the ionization of donor states located near the semiconductor interface. The donor electrons then can contribute to electrical conductivity and the presence of ions can be indicated by the change in current, capacitance or resistivity depending on the device design.

It should be noted that today it is possible to dope the material in a controlled way and to tailor the electronic properties of semiconductors that leads to the creation of new functional electronic devices.

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ԴՈՆՈՐԱՅԻՆ ՎԻՃԱԿՆԵՐԻ ՖԻԶԻԿԱԿԱՆ ՀԱՏԿՈՒԹՅՈՒՆՆԵՐԸ ԿԻՍԱՀԱՂՈՐԴՉԻ ՄԵՐՁՄԱԿԵՐԵՎՈՒԹԱՅԻՆ ՏԻՐՈՒՅԹՈՒՄ` ԱՐՏԱՔԻՆ ԷԼԵԿՏՐԱԿԱՆ ԴԱՇՏՈՒՄ

Վարիացիոն եղանակով հետազոտվել են կիսահաղորդչի մերձմակերևութային տիրույթում տեղայնացված դոնորային խառնուրդի հիմնական վիճակի էներգիան և ալիքային ֆունկցիան` տեսածրող թունելային մանրադիտակի սայրով ստեղծված էլեկտրական դաշտում: Ցույց է տրվել, որ սայրի դրական պոտենցիալի դեպքում կատարվում է դոնորային կենտրոնի իոնացում: Քննարկվել է ստացված արդյունքների հիման վրա նոր տիպի գազային դետեկտորների ստեղծման հնարավորությունը:

Առանցքային բառեր. դոնորային վիճակներ, մերձմակերևույթ, թունելային մանրադիտակի սայր:

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ФИЗИЧЕСКИЕ СВОЙСТВА ПРИПОВЕРХНОСТНЫХ ДОНОРНЫХ СОСТОЯНИЙ В ПОЛУПРОВОДНИКЕ ВО ВНЕШНЕМ ЭЛЕКТРИЧЕСКОМ ПОЛЕ

Вариационным методом исследованы энергия и волновые функции нейтрального донора, локализованного вблизи поверхности полупроводника во внешнем электрическом поле, созданном металлическим острием сканирующего туннельного микроскопа (СТМ) или металлическим шариком. Показано, что при положительном напряжении на острие СТМ происходит ионизация донора. Обсуждена возможность применения полученных результатов для создания нового типа газовых детекторов.

Ключевые слова: донорные состояния, интерфейс, острие сканирующего туннельного микроскопа.