Armenian Journal of Physics, 2014, vol. 7, issue 1, pp. 38-49

BEHAVIOR OF A SHALLOW DONOR BINDING ENERGY NEAR A SEMICONDUCTOR SURFACE IN THE PRESENCE OF SCANNING TUNNELING MICROSCOPE TIP

A.P. Djotyan

Yerevan State University, Dept. of Physics, A. Manoogian 1, Yerevan, 0025, Armenia

Received 5 December 2013

Abstract – The ground state energy and the extend of the wavefunction of a neutral donor located near a semiconductor surface in the presence of a STM metallic tip held at a fixed potential is obtained within a variational approach. We apply the effective mass approximation and use a variational wavefunction that takes into account the influence of all image charges that arise due to the presence of a metallic tip. The latter lowers the shallow donor energy which is lower than in the case when the donor is located at the same distance near a plane semiconductor-metal interface. The ionization process of a donor center due to the tip positive voltage is considered. In the case of negative voltage on the tip we observe a nonmonotonic behavior of the impurity electron binding energy.

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

1. INTRODUCTION

Dopant atoms are essential in semiconductor technology since they provide extrinsic charges necessary to create devices such as diodes and transistors. The possibility to dope the material in a controlled way and to tailor the electronic properties of semiconductors has led to the creation of new functional electronic devices and to recent proposals for e.g. quantum cellular automata [1] and single electron transistors [2]. A full spatial control of the incorporation of single P dopant atoms in Si (001) was realized in Ref. [3] which opens a new avenue for the creation of atomic-scale electronic devices. An example is the proposal of Kane [4] to use donor states as qubits. Due to further downscaling in microelectronics the effect of the boundary on such impurity states have become a problem of fundamental interest [5, 6], and the dopant atoms appear closer and closer to interfaces [7, 8].

Resonant tunneling between source and drain of a gated nanowire was used in Ref [5] to realize the spectroscopy of a single dopant atom in silicon. The electronic states of this dopant appeared as resonances in the low temperature conductance at energies below the conduction band edge. While the first resonance is consistent with the binding energy of the neutral D^0 state of an arsenic donor the second one demonstrated a reduced charging energy due to the electrostatic coupling of the charged D^- state with the electrodes.

A more direct and flexible technique to investigate dopant atoms close to the surface is offered by the method of scanning tunneling microscopy (STM). The electrostatic potential induced by the tip allows to manipulate the charge state of individual impurities near the surface of the semiconductor [7]. The manipulation was fully controlled by the position of the tip and the voltage applied between the tip and the sample. The STM experiments were performed at low temperature on the 110 surface of silicon doped GaAs. Silicon donors up to 1 nm below the surface could be reversibly switched between their neutral and ionized state by the local potential induced by the tip. In Ref. [8] the typical depth of the investigated donor was about 1.2 nm. The tip was electrochemically etched tungsten with a radius of curvature of the apex of a few nanometers. From these experiments it is clear that the binding energy of an electron to the donor

will be influenced by the semiconductor-vacuum interface and the presence of the metallic STM-tip.

The energy spectrum of a donor located near a plane semiconductor/metal interface was investigated in Ref. [9] using the finite element technique. In our previous work [10] we investigated the lowest electronic states of a donor located near a semiconductor-insulator-metal plane interface within the effective mass approximation. The lowest energy states were obtained 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, and the results were compared with a numerical exact calculation using the finite element technique and good agreement was obtained. Our previous results [10] for a semiconductor-dielectric interface (which was based on a variational wave function with only 3 variational parameters) are very close to the corresponding ones found by MacMillan and Landman [11] who used the variational method with a trial wavefunction consisting of a summation over a basis set of wave functions.

The ground state energy of a donor localized near a semiconductor/dielectric interface (in Si near a thick insulating layer) was also studied in Ref. 12 using a variational approach.

In this paper we investigate the effect of the presence of a STM metallic tip (which we approximate by a sphere) on the donor binding energy and the electron wavefunction when a neutral donor is placed near a semiconductor-vacuum surface.

In the s-wave-tip model of the STM tip suggested in Ref.13 and Ref. 14 the tip was modeled as a protruded piece of metal, with a radius of curvature a [15]. Probe tip can be of arbitrary shape but is assumed locally spherical where it approaches to the semiconductor surface. The solutions of the Schrödinger equation for a spherical potential well of radius a were taken as tip wave functions. Corresponding theoretical calculations [13,14] were in excellent agreement with experimental results.

Therefore, it was shown that only the distance of the center of curvature of the tip to the sample surface is important.

In accordance with the theory of scanning tunneling microscope developed in Ref.13 and Ref.14 we approximate the tip by a metallic sphere with the radius a.

The behavior of the ground state energy when the grounded tip approaches the semiconductor surface is investigated in Ref.16. There we considered the vertical (perpendicular to the semiconductor surface, on OZ-direction) and lateral (on the semiconductor surface, i.e. on OX- and OY- directions) motion of the metallic sphere, and therefore modeling the scanning motion of the STM tip.

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.

In the calculations of the impurity energy spectra we take into account all image charges of the electron and the donor center which arise in a grounded or charged metallic tip, i.e. in the cases of zero or nonzero constant potential on the tip. As in Ref.16, our approach is based on the effective mass theory and does not include effects due to e.g. structural deformations of the surface because of the presence of the donor. Therefore, our results are valid only for donor atoms which are situated at least several monolayers below the surface.

This paper is organized as follows. In Sec.2 we present our model, the underlying theory and discuss the variational wave function. This section gives also the expression that determines the neutral donor energy near a semiconductor surface in the presence of a STM tip (approximated by a metallic charged sphere) in closed analytical form. In Sec.3 and Sec.4 we present our numerical results and discussions. Our conclusions are presented in Sec.5. The interpretation of the electric field potential created by the donor near a semiconductor plane surface in the vicinity of a metallic grounded sphere is given in the Appendix.

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. As in [16], 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 $a_B^* = \hbar^2 \varepsilon / m_e e^2$ and the 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 [17,18].

2.2 The vertical position of the tip

Firstly 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.

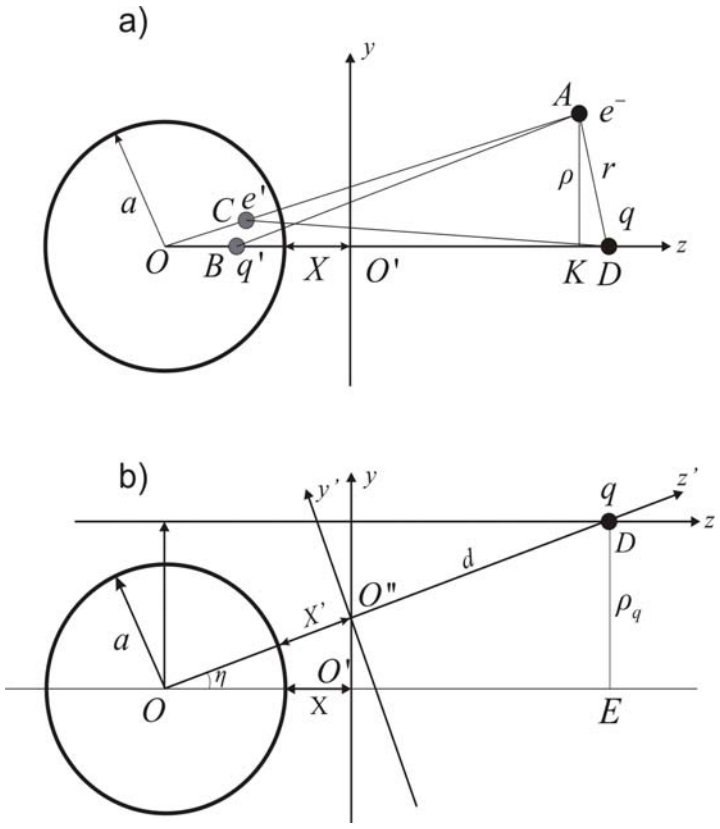

Figure 1. Schematic picture of the system configuration in the case when the tip:
(a) is placed on top of the donor; (b) is shifted (non-central) laterally with respect to the donor. The donor is positioned at point D.

The potential energy of the impurity electron (with the charge $-e$) at point *A* near of 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 V is the same as in the case of neutral tip considered in Ref.16 except that now the charge $ne = Va$ with $(n = \pm 1, 2..)$ should be placed in the center of the sphere [17]. So, the corresponding equation for the potential energy of the electron becomes

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

where $e' = ea / OA$ is the electron image which arises at point C at distance $OC = a^2 / OA$ from the tip center; the donor image $q' = -ea / OD$ is located at point B at distance $OB = a^2 / OD$ from the center of the tip [17,18]. 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 added term n / OA in Eq. (6) describes 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 corresponding distances: the distance CA between the electron and its image is

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

the distance BA between the electron and 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 $OD = a + X + d = a' + d$ is the donor-tip center distance with X being the interval between the tip and the semiconductor surface.

In dimensionless units expressed in terms of the Bohr radius and twice the 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 used in Ref. 16, where we modified the exponential factor $\exp(-\beta z)$, which describes the influence of the images on the electron, to the $\exp(-\beta CA)$:

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

and $r = AD = \sqrt{\rho^2 + (z - d)^2}$. 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

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

$$\psi H\psi = \psi^2\left(\frac{\lambda}{r}(1+\beta k_2(k-2)+\frac{z-d}{z})-\frac{\lambda^2+\beta^2(k-2)^2}{2}+\frac{\beta}{OA}(1-\frac{OK}{z}(k-2))+U_{Coul}\right), \quad (7)$$

where $k = CA/OA$, $k_2 = ((z-d)OK+\rho^2)/OA$ and $OK = a'+z$.

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 [7,8].

The tip at a positive voltage $(n=-1,2..)$ gives rise to a positive shift in the energy, and when this shift is equal to the binding energy, then the state becomes resonant with the conduction band in the bulk and the donor ionizes. The magnitude of this shift was estimated in Ref. 8 by the overlap between the wave function of the donor and the tip induced band bending using a 1*s* wave function. 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 with the potential energy given by Eq. (1) using the wave function given by Eq. (5).

2.3 The lateral position of the tip

Now we consider the more general case where the tip is shifted laterally (e.g. in *y*-direction). In this case the donor is displaced from the axis *OE* (previous *OZ* axis, which passes through the tip center perpendicularly to the semiconductor surface). Now we take the line *OD* passing through the center of the tip and the donor location point *D* as the new *OZ′*-axis with point *O″* (see Fig. 1b) as the origin of a new system of cylindrical coordinates. Notice that now the new *OZ′*-axis is not perpendicular to the semiconductor surface. The position of the electron in this coordinate system is described by the variables (ρ, z, θ); the shifted position of the donor is described by the parameter $\rho_q = a+y$ (the distance of the donor from the axis *OO′*, where y is the distance from the tip surface to the *OZ*- axis).

The potential energy between the electron at the point A (with the charge −e) and the donor impurity (with the charge $q=e$) located at the point *D* near the metallic grounded sphere (a tip) with the radius a is given again by Eq. (1) but now with the new expressions for the corresponding distances; η is the rotation angle between the corresponding axis *OY (OZ*) and *OY′ (OZ′)*

$$\tan\eta = \frac{\rho_q}{a+X+d};\ \rho_q = a+y. \quad (7)$$

We choose the ground state variational wave function ψ of the system in the following form:

$$\psi = N\, I(\mathbf{r})\exp(-\beta CA)\exp(-\lambda r), \quad (8)$$

where the function $I(\mathbf{r})$ is the distance between the electron and the semiconductor interface.

Notice that the boundary condition is changed from $\psi\ (z=0)=0$ to $\psi\ (I(\mathbf{r})=0)=0$. In the new coordinate system we have $I(r) = z\cos(\eta)-\rho\sin(\eta)\sin(\theta)$.

3. Negatively charged tip

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 dependences for the average positions $< z - d >$ and $< \rho >$ are shown in Fig. 2b.

The positive shift in the energy is determined by the sum of two positive terms in the potential energy Eq. (1): the first is due to image charges and is proportional to $a/(a + x + d)^2$ (for values of $a/(a + x + d) \sim 1$) while the second one arises due to the charge on the tip and is proportional to $1/(a + x + d)$. The influence of the image term is much smaller in comparison with the charged tip term and therefore the second term is crucial for the donor ionization.

In the case of an uncharged tip $(n = 0)$, for the values of the parameters $d = 1, x = 1.1, a = 0.2a_B$ the account of the image charges leads to a decrease of the system energy (in units of $2Ry$) from $E' = -0.301$ to $E = -0.2837$ (the decrease is about 5%). The application of the potential on the tip $(n = -1)$ leads to a drastic decrease of the energy, it becomes $E' = -0.017$ (for the same values of the charged tip term and therefore the second term is crucial for the donor ionization.

In the case of an uncharged tip $(n = 0)$, for the values of the parameters $d = 1, x = 1.1, a = 0.2a_B$ the account of the image charges leads to a decrease of the system energy (in units of $2R^*$) from $E' = -0.301$ to $E = -0.2837$ (the decrease is about 5%). The application of the potential on the tip $(n = -1)$ leads to a drastic decrease of the energy, it becomes $E' = -0.017$ (for the same values of the parameters and in the absence of the image charges). The account of the image charges leads to a further decrease of the energy, i.e. the energy becomes practically zero and the donor is ionized.

It is clear that for 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. 8a, 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 $X_c = 1.1$. However, as seen in Fig. 2b, the average distances $< \rho(d) >$ and $< z - d >$ > for $a = 0.5a_B$ are smaller than the corresponding ones for $a = 0.2a_B$.

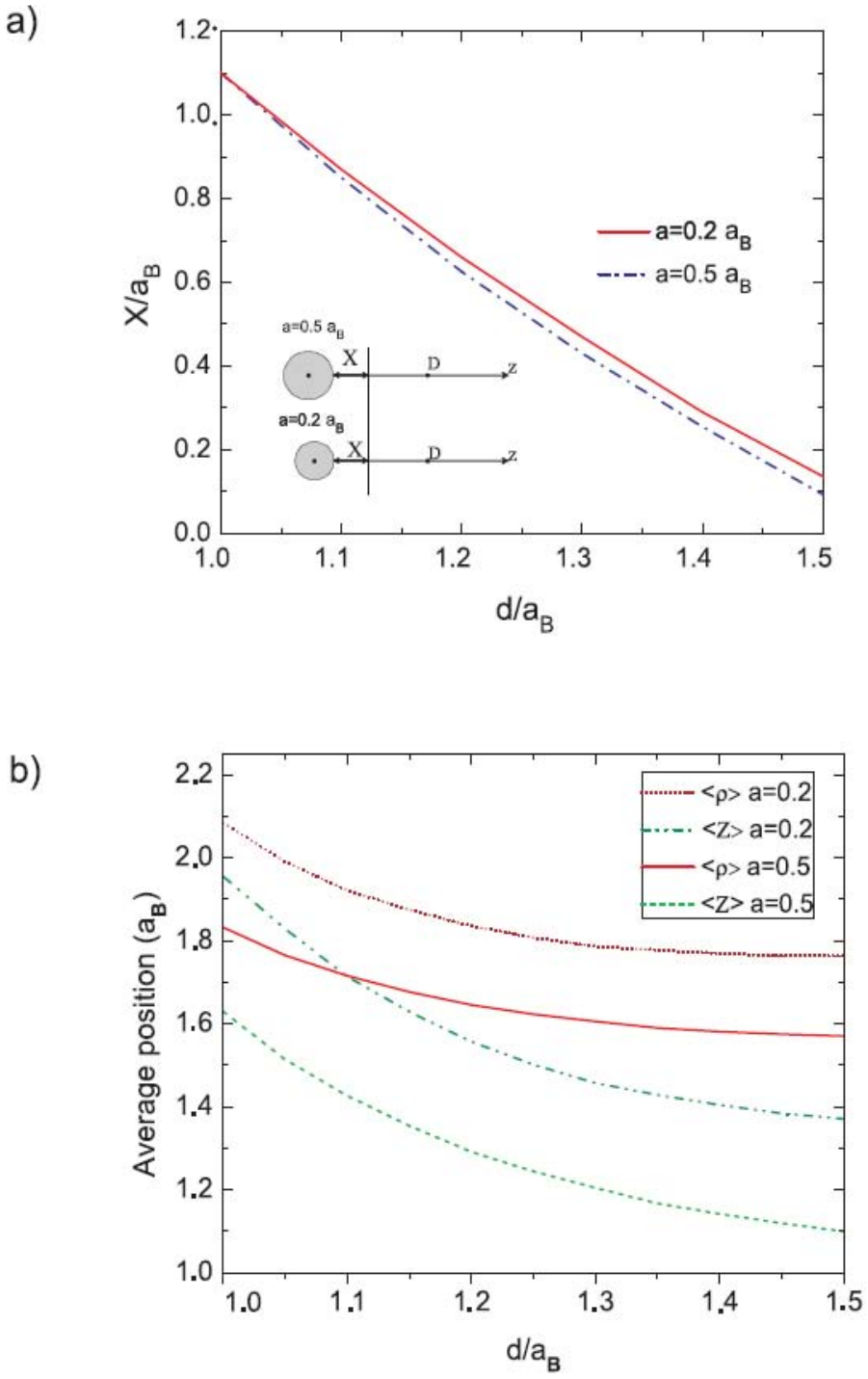

Fig. 2: a) The dependence for the critical value of the tip-semiconductor distance X for donor ionization (for two different values of the tip radii $a = 0.5a_B$ and $a = 0.2a_B$) on d when the charge of the tip is $-e$ (i.e. $n = -1$). Inset: schematic representation of the studied systems; b) The corresponding 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 $10^{-3}(2R^*)$.

This difference in the electronic configurations can be explained as follows. The situation here differs radically from the case of a neutral tip described in Ref.16 (see Fig.5 in Ref.16). Now, when the impurity center is almost ionized due to the charge on the tip, the electron is mostly bound by its image as it was for a plane gate with the screened Coulomb potential

$U = -1/4z$ [10]. Due to the stronger attraction of the electron by its image in the case of a larger tip (with $a = 0.5a_B$) the average distances are smaller in comparison with the case of a smaller tip (with $a = 0.2a_B$). Notice that the electron charge distribution is not spherical and is more spread out towards the interface for the case of a larger tip (the relative difference between the $<\rho(d)>$ and $<z-d>$ values at $d=1$ for $a = 0.5a_B$ is about 10% while it is 7% for $a = 0.2a_B$).

4. Positively charged tip

In the case when a negative voltage for the impurity electron (i.e. negative potential energy) is created by the positively charged tip, we obtained a strong lowering of the ground state energy as shown in Fig. 3. The reason is that the electron is now attracted also by the positive charge placed in the center of the tip. The behavior of the system energy in this case crucially depends on the donor distance *d* from the semiconductor surface. Fig. 3 shows that for $d = a_B$ the energy of the system (in the case of positive charge e on the tip) monotonically decreases with decrease of ρ_q, while for $d = 0.5a_B$ the ground state energy has a nonmonotonic dependence. Such dependence can be explained as follows. In the absence of the tip the averages in ρ and z directions are about $2a_B$ for $d = 0.5a_B$ (for $X = 0$), which shows that the electron distribution is strongly spread out on the interface. Due to this the charged (with *e*) tip approaching to the donor (with $d = 0.5a_B$) in lateral direction strongly interacts with the electron at intermediate values of the tip-donor lateral distance $\rho_q = 1.5a_B$, resulting in the energy lowering as shown in Fig. 3.

Indeed, Fig. 4 shows that for $\rho_q = 1.5a_B$ the electron expectation value $<\rho> = 1.5a_B$, indicating that the electron is just ”in front” of the tip.

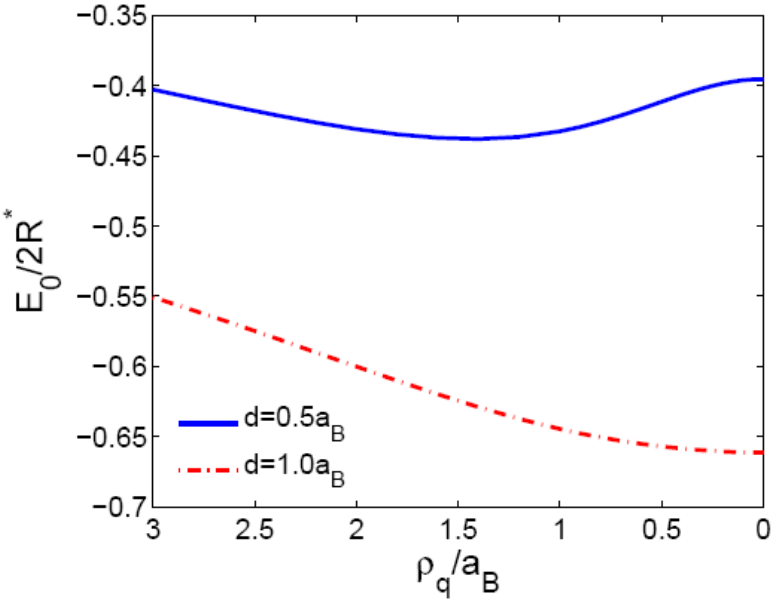

Fig. 3: The energy of the ground state of an impurity electron as a function of the tip-donor lateral distance ρ_q for different distances of the donor from the interface for the case of the negative voltage on the tip.

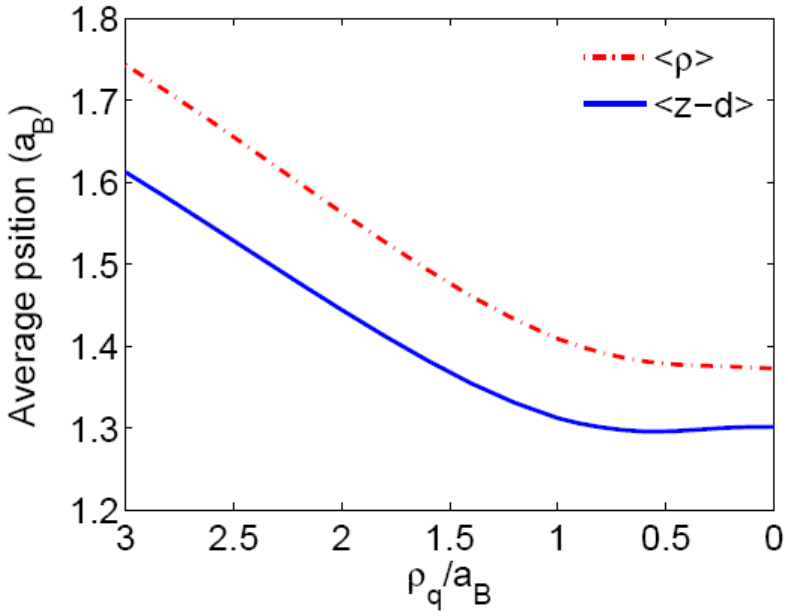

Fig. 4: Average positions of the impurity electron in the ρ and z-directions for $d = 0.5a_B$ as a function of the tip-donor lateral distance ρ_q.

For the region of $a_B < \rho_q = 2a_B$ the electron distribution is prolonged to the tip, so the electron is being localized between the tip and the donor. This electron configuration, i.e. the electron is bound with both of the positive centers, is similar to that in a molecule with inter-nuclear distance about $1.5a_B$. When the tip approaching the donor closer (i.e. when $\rho_q < 1.5a_B$) the energy becomes shallower (see Fig. 3). This is due to fact that: i) the interface strongly repeals the electron from the donor and ii) the position of the positively charged centers is shifted from the equilibrium one which gives the energy minimum. So, we obtain a nonmonotonic dependence for the energy with minimum at $\rho_q \approx 1.5a_B$, where the tip effectively attracts the electron.

As shows Fig. 4, for the case when $d = a_B$ the average values dependences on ρ_q are more flat.

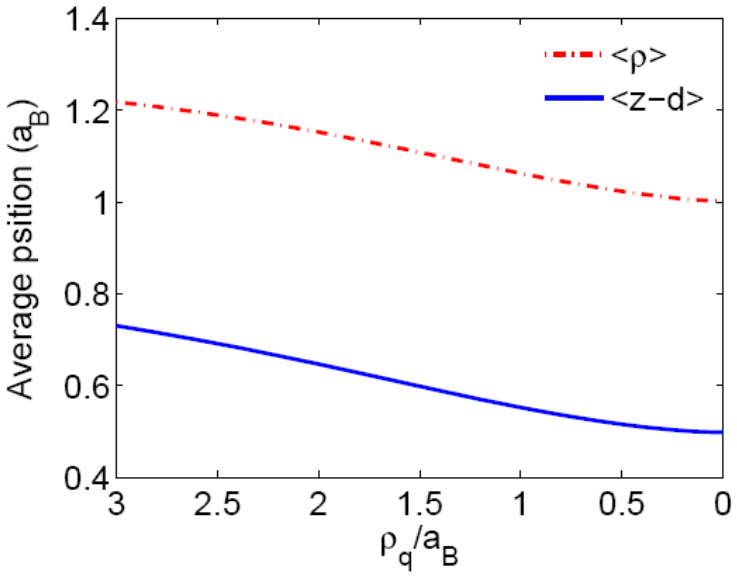

Fig. 5: Average positions of the impurity electron in the ρ and Z directions as a function of ρ_q for the donor-interface distance $d = a_B$.

For this case the repulsive effect of the interface is weaker and the electron is not spread on the interface as in the case $d = 0.5a_B$. So, for the distance $d = a_B$ the system reaches its lowest value of the energy at $\rho_q = 0$, i.e. at vertical position of the tip.

5. CONCLUSION

In this paper we investigated the influence of a STM metallic tip on the ground state energy of an impurity located near a semiconductor surface. We obtained the donor binding energy and its dependence on the tip radius and the distance between the donor and the semiconductor surface using a variational approach. The proposed trial variational function takes into account all correlations between the particles and its images.

We have investigated the ionization of the donor due to a positive voltage on the tip (positive energy for impurity electron - tip interaction created by a negative charge on the tip).

In the case when a negative voltage for the impurity electron (i.e. negative potential energy) is created by the positively charged tip, we obtained a strong lowering of the impurity electron ground state energy. We observed a nonmonotonic behavior of the binding energy for some positions of the donor ($d = 0.5a_B$) when the tip laterally approaches to the donor.

Appendix A

In this appendix we consider the symmetry properties of the electric field potential created by the impurity electron (when the donor is located near a semiconductor surface) in the presence of the STM metallic tip. We will show that the potential energy of the interaction of the electron with the donor image (as in the case of a plane semiconductor/metal interface) is equal to the one between the electron image and the donor.

Let us start from a plane metal/semiconductor problem with the donor placed near a grounded metallic plane at position (0, d). From a mathematical point of view we have to solve Poisson's equation in the region z > 0, in the presence of a single point charge *q* at *(0, d)*, subject to the boundary conditions $V = 0$ for $z = 0$ (since the conducting plane is grounded), and $V = 0$ far from the charge. The uniqueness theorem guarantees that there is only one function that meets these requirements.

The potential created by the donor near the metallic plane (in cylindrical coordinates with the center on the plane) can be described by the image charge method, namely

$$V = \frac{e^2}{\varepsilon}\left[\frac{1}{\sqrt{\rho^2 + (z-d)^2}} - \frac{1}{\sqrt{\rho^2 + (z+d)^2}}\right], \tag{A1}$$

and it satisfies the correct boundary conditions (V=0 when z=0 and V=0 far from the charge).

When we bring the electron from infinity to the interface the potential energy of the electron becomes:

$$U_{Coul} = \frac{e^2}{\varepsilon}\left[-\frac{1}{4z} - \frac{1}{\sqrt{\rho^2 + (z-d)^2}} + \frac{1}{\sqrt{\rho^2 + (z+d)^2}}\right]. \tag{A2}$$

We added in Eq. (A1) the term $-e^2/4z\varepsilon$ which describes the interaction of the electron with its image which are separated by a distance $2z$. This term has an extra coefficient *2* in the dominator, since the work is zero when the image of the electron is moved in the metal towards the interface [18]. We can interpret the third term as the result of the interaction between one particle (electron or impurity) and the image of the other particle (impurity or electron image charge). Alternatively, we can interpret the third term as the sum of two equal terms, each one with coefficient 1/2 ; the first one describes the interaction between the electron and the donor

image and the second one describes the interaction of the donor with the electron image. This potential energy can be obtained if one brings the donor and the electron simultaneously from infinity to these final positions near the interface. In the case when the donor is located near a semiconductor plane surface in the vicinity of a metallic grounded sphere, the potential of the electric field created by the electron can be found using the method of images [17, 18] (see Sec. 2):

$$U^{*}_{Cool} = e^2 / \varepsilon\left[-a / 2OA \cdot CA + a / OD \cdot AB - 1 / AD\right]. \qquad \text{(A3)}$$

As we see, for the tip problem (see Fig. 1), the distance *AB* from the electron to the donor image and the distance *CD* from the donor to the electron image are not equal. But it is easy to see that (as in the case of a plane metal) the two potential energies $U = -eq'/2AB$ (between the electron and the donor image) and $U = -eq'/2CD$ (between the donor and the electron image) are equal. The triangles *OAB* and *OCD* are similar because they have a common angle *AOD* and we have also *OC/OB = OD/OA* (from the electrostatic's condition) so we have that *OC/OB = OD/OA = CD/AB*. This relation leads to the potentials
$U_1 = -eq'/2AB = -eqa/2AB \cdot OD$ and $U_2 = -eq'/2CD = -eqa/2CD \cdot OA$ which are equal to each other because *AB · OD = CD · OA*. So, Eq. (A3) becomes:

$$U_{Cool} = 1/\varepsilon\left[-ee'/2CA - eq/AD - eq'/2AB + e'q/2CD\right].$$

Acknowledgements

I thank Prof. F.M. Peeters and Dr. A.A.Avetisyan for fruitful discussions and valuable remarks.

References

[1] G. L. Snider, A. O. Orlov, I. Amlani, X. Zuo, G. H.Bernstein, C. S. Lent, J. L. Merz, and W. Porod, J. Appl. Phys. 85, 4283 (1999).
[2] J. R. Tucker and T. C. Shen, Int. J. Circuit Theory Appl. 28, 553 (2000).
[3] S. R. Schofield, N. J. Curson, M. Y. Simmons, F. J. Rueß, T. Hallam, L. Oberbeck, and R. G. Clark, Phys. Rev. Lett. 91, 136104 (2003).
[4] B. E. Kane, Nature (London) 393, 133 (1998).
[5] H. Sellier, G. P. Lansbergen, J. Caro, S. Rogge, N. Collaert, I. Ferain, M. Jurczak, and S. Biesemans, Phys. Rev. Lett. 97, 206805 (2006).
[6] Kuan Yen Tan, Kok Wai Chan, Mikko Mttnen, Andrea Morello, Changyi Yang, Jessica van Donkelaar, Andrew Alves, Juha-Matti Pirkkalainen, David N. Jamieson, Robert G. Clark and Andrew S. Dzurak, Nano Lett. 10, 11 (2010).
[7] K. Teichmann, M. Wenderoth, S. Loth, R.G. Ulbrich, J.K. Garleff, A.P. Wijnheijmer, and P.M. Koenraad, Phys. Rev. Lett. 101, 076103 (2008).
[8] A. P. Wijnheijmer, J. K. Garleff, K. Teichmann, M. Wenderoth, S. Loth, R. G. Ulbrich, P. A. Maksym, M. Roy and P. M. Koenraad, Phys. Rev. Lett. 102, 166101 (2009).
[9] A.F. Slachmuylders, B. Partoens, F.M. Peeters, andW. Magnus, Appl. Phys. Lett. 92, 083104 (2008).
[10] Y. L. Hao, A. P. Djotyan, A. A. Avetisyan, and F. M. Peeters, Phys. Rev. B 80, 035329 (2009); ibid. Phys. Rev. B 83, 199904(E) (2011).
[11] D.B. MacMillen and U. Landman, Phys. Rev. B 29, 4524 (1984).
[12] M.J. Calder´on, B. Koiller, and S. Das Sarma, Phys. Rev. B 75, 125311 (2007).

[13] J.Tersoff, and D.R.Hamann, “Theory and application for the scanning tunneling microscope,”Phys. Rev. Lett, 50, 1999 (1983).
[14] J.Tersoff, and D.R.Hamann, Phys.Rev B, 31, 805 (1985).
[15] J.C.Chen. Introduction to Scanning Tunneling Microscopy. Second Edition, Oxford University Press (2008).
[16] A. P. Djotyan, A. A. Avetisyan, Y. L. Hao, and F. M. Peeters. Proc. SPIE, 8414, 84140L (2011)
[17] J. D. Jackson, Classical Electrodynamics. 3rd ed., John Wiley & Sons Press, New York, 1998.
[18] D. J. Griffiths, Introduction to Electrodynamics. 3rd ed., Prentice Hall, New Jersey, 1999.