# DETERMINATION OF THE ELECTRON AFFINITY (WORK FUNCTION) OF SEMICONDUCTOR NANOCRYSTALS

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We present a new method of determination of electron affinity  $X_0(L)$  of semiconductor nanocrystals with various lattice constants L that takes into account the experimental (or calculated) data on the forbidden gap width  $E_g(L)$  and the relation:  $E_g(L) + X_0(L) = 5.5 - \Delta E_{gv}(L) \approx 5.5$  eV. This relation is proposed to use for bulk and quantum-sized structures. Its detailed verification for a number of semiconductor cubic crystals is performed.

### 1. Introduction

In the previous works [1–4], a method of determination of the band parameters of semiconductor crystals with (diamond-like) fcc lattices, namely the forbidden gap width  $E_g$ , valence band energy  $E_v$ , conduction band energy  $E_c$ , melting temperature, etc., as functions of the well-known parameter – crystal lattice constant L or the quantity proportional to it, the minimum interatomic distance d. Both last quantities are determined by the sum of valence radii of neighboring atoms,  $d = (r_a + r_b)$ , forming the crystal lattice, i.e. by the first coordination sphere radius. For many crystalline compounds, the quantity L is available from the handbooks and can be calculated with sufficient accuracy with the use of tabular values of the valence radii of elements. In particular, for the tetrahedral configuration of a cell (i.e. for diamond-like fcc lattices) in the case of onecomponent crystals (formed from elements of groups III–V of the Periodic table),  $L = 4kr_a/\sqrt{3}$ ; for two-component crystals,  $L = 2k\frac{(r_a+r_b)}{\sqrt{3}}$ , etc. These quantities are determined to within the coefficient  $k \approx 0.9$  which accounts a small decrement of the valence radii on the joining of atoms into a molecule abo under condensation |5-8|.

In those works, it was shown that the band parameter, the forbidden gap width  $E_g$ , is also related to the value of electron affinity (or the emissive work function)  $X_0$ . Thus, by setting  $E_g(L)$ , one can obtain the corresponding values of  $X_0$ . In what follows, we consider this problem for ordinary "bulk" crystals and for nanocrystalline bodies, where the band parameters are changed due to the quantum-size mechanisms.

# 2. Analysis of Band Parameters for Bulk FCC Crystals

The results of works [1–8] testify that the properties of crystalline bodies are genetically programmed in such a parameter of atoms as the radius of an external (valence) orbital. In order to unambiguously describe the behavior of band parameters of crystals, the analysis of components of the binding energy as functions of the base parameters of atoms forming a solid such as the energies of valence  $E_v$ , metallic  $E_m$ , and ionic  $E_i$  couplings was carried out in [2–4].

These components are calculated with sufficient accuracy in the approximation of strong coupling (LCAO), by using the energy terms of external electron orbitals  $\varepsilon_s$  and  $\varepsilon_p$  [3–8] available from the handbooks as tabular data [9, 10]. For the collectivized states (the atom-molecular or condensed state), they are different due to the Pauli principle, and  $\varepsilon_s > \varepsilon_p$ . As known, this leads to the appearance of the bands of free (excited) electrons,  $E_c$ , and bound (valence)  $E_v$  electrons.

The value of valence energy  $E_v$  is easily calculated in terms of the lattice constant and coincides with the tabular value [5–8]. In this case, it is necessary to take two following effects into account:

1) Hybridization of the orbitals which firm the chemical, including valence, coupling with the effective energy term  $\varepsilon_h = \frac{1}{4}(\varepsilon_s + 3\varepsilon_p)$  (in the case of the  $sp^3$ -hybridization). The solutions of the Schrödinger equation for bound atoms give two values of energy: the lower value that corresponds the bonding action,  $E_b = \varepsilon_h + E_v$ , and the higher one corresponding to the the antibonding action  $E_{ab} = \varepsilon_h - E_v$ . The difference between these values is related to the valence component of forbidden states.

2) Appearance of the metallic coupling which has antibonding (repulsive) character due to the screening

of the valence coupling (exchange interaction). This mechanism is quantitatively characterized by the difference of the terms  $E_m = \frac{1}{2} (\varepsilon_s - \varepsilon_p)$ . The analysis of the values of  $E_m (L)$  for many semiconductor crystals [4] indicates that this difference of energies  $(\varepsilon_s - \varepsilon_p)$  is almost constant, as distinct from its strongly varying components  $\varepsilon_s(L)$  and  $\varepsilon_p(L)$ . Thus, irrespective of the absolute values of  $\varepsilon_s(L)$  and  $\varepsilon_p(L)$ , the energy of metallic coupling in the LCAO approximation can be considered constant with an accuracy of  $\approx 10\%$ . Namely,

$$E_m = 2.2C_m, \quad C_m = \left[1 - \frac{(L - L_D)}{4L_D}\right],$$

$$E_m \approx (1.9 \pm 0.2) \text{ eV}.$$
 (1)

The energy of attractive coupling, in addition to the valence (exchange) component, has else the polar component.

For the valence component, its dependence on L was established in the classical works [5–8]. It decreases monotonously (with increase in L) and has shape of a square parabola:

$$E_V = A/L^2, \quad A = 7.8 \cdot L_D^2 [eV/Å^2],$$
 (2)

where  $L_D$  is the lattice constant of diamond.

The ionic component arises only in the case of nonidentical atoms in the crystal at the expense of an asymmetric redistribution of the density of the electron clouds of neighboring atoms which create the chemical coupling. Thus, this component is defined as the difference of the electron terms of neighboring atoms:

$$E_i = \frac{1}{2} \left( \varepsilon_a - \varepsilon_b \right). \tag{3}$$

Since the reconstruction (the so-called hybridization) of atomic orbitals occurs on the formation of interatomic chemical bonds, it is necessary to use the hybrid terms which can be obtained with the eligible accuracy in the linear approximation:

$$\varepsilon_h(sp^3) = \frac{1}{4} \left( \varepsilon_s + 3\varepsilon_p \right), \quad \varepsilon_h(sp^2) = \frac{1}{3} \left( \varepsilon_s + 2\varepsilon_p \right),$$
$$\varepsilon_h(sp) = \frac{1}{2} \left( \varepsilon_s + \varepsilon_p \right). \tag{4}$$

Then the energy of ionic coupling reads

$$E_i = \frac{1}{2} \left( \varepsilon_{ha} - \varepsilon_{hb} \right). \tag{5}$$

This difference, as distinct from the energy of metallic coupling, depends quite strongly on the lattice constant. Like the energy of valence coupling, it decreases with increase in the lattice constant by the sharper power law:

$$E_i \approx B_i/L^n, \quad n \sim 2 \div 3.$$
 (6)

Moreover, the coefficient  $B_i$  remains invariant only for the sets with common cathode under changing the elements of the which belong to the same column of the Periodic table.

The other simple method of calculation of  $E_i$  does not require the data on  $\varepsilon_h$  and consists in the use of the tables of the electronegativies of elements by Pauling  $X_A, X_B$ , and  $X_C$ . Namely, the difference  $\Delta X = X_a - X_b$ sets the coupling ionicity degree:  $\alpha_i \approx \frac{1}{2}\Delta X$ . Hence,

$$E_i \approx \alpha_i E_v \approx \frac{1}{2} \Delta X E_v. \tag{7}$$

For one-component materials,  $\Delta X = 0$ . In this case, the ionic coupling is absent. It is also small for anode– cathodic compounds with close position in the Periodic table of elements and a small value of  $\Delta r = r_a - r_b$ , i.e. with a small dipole moment for basic polarized atoms.

Thus, using the relation for three calculated components of the binding energy in the crystal state, we obtain the general analytic formula for the binding energy of a valence electron in the crystal under its excitation to the conduction band. That is, we get the forbidden band width as a function of the lattice constant L:

$$E_{g\Sigma} \approx E_{gvD} \left(\frac{L_D}{L}\right)^2 \left(1 - k \left(\frac{L}{2L_D}\right)^2\right) \left(1 + \alpha_i^2\right)^{1/2}.$$
(8)

Here, the normalizing constant  $E_{gvD} = 7.8$  eV is the valence component of the forbidden band of diamond,  $k \approx 1.2$  is the correction concerning the degree of approximation of the LCAO calculation, and  $E_{gD} = 5.5$  eV.

In Figs. 1–3, we show the experimental forbidden band widths  $E_g$  for many cubic semiconductors with a small share of polar coupling (at most 20%) versus the lattice constant L and the theoretical curves constructed by the last formula.

In order to calculate the work function (electron affinity)  $X_0$  and its dependence on the lattice constant L, we consider the earlier obtained dependence of the band spectrum on L [5–8] (see Fig. 1). It is seen that,

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Fig. 1. Band energy vs lattice constant for cubic fcc crystals of group IV

for crystals of group IV of the Periodic table, the energy of the excited band is connected with  $X_0$  by the analytic relation

$$E_q + X_0 = 5.5 - \Delta E_v \approx \text{const},\tag{9}$$

 $\Delta E_v = (1 - kL/2L_D)$ ,  $\Delta E_v = (0 \div 0.6)$  eV is a change in the edge of the valence band.

Let us assume that a similar relation holds also for other groups of diamond-like (fcc) crystals (i.e. the influence of ionic components of the coupling is neglected). Then we get the following relation for the electron affinity (i.e. the barrier for the emission of electrons into vacuum):

$$X_0^{(L)} = 5.5 \left[ 1 - 1.4 \left( L_D / L \right)^2 \left( 1 - \left( \frac{L}{2L_D} \right)^2 \right) \right] - \Delta E_v.$$
(10)

That is, the dependence of the emissive work function (electron affinity)  $X_0$  on L is presented in the analytic form, and it is antisymbatic to the dependence  $E_g(L)$ . This relation is demonstrated in Fig. 2 for many crystals

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Fig. 2. Valence matrix element (1) and forbidden band width (2– 4) vs lattice constant L. (2 – for semiconductors with a large share of ionic coupling, 3 – with a low share of ionic coupling, and 4 – without ionic coupling)

of group IV and for crystals with low share of ionicity. The theoretical curves are compared with the experimental data and with the new data considered in this work. It is seen that the work function  $X_0$  grows with L up to the maximum value. For semiconductor crystals, it is  $X_{0\text{max}} \approx 5$  eV. At the same time, the sum  $E_g + X_0$  is almost constant  $\approx 5.5$  eV, according to relation (10). As seen from Fig. 2, by changing the composition of fcc crystals (Si<sub>x</sub>C<sub>1-x</sub>, Si<sub>x</sub>G<sub>1-x</sub>, cubic Si<sub>x</sub>Sn<sub>1-x</sub>, etc.), one can easily vary the work function in a quite wide range (from 0.4 to 4 eV).

## 3. Analysis of Band Parameters for Nanosized Crystals

In quantum-size nanocrystals, it is possible to significantly increase the forbidden band width and the binding energy of excitons. The last quantity can essentially influence the results of calculations of the dimensional quantization energy. Therefore, it is necessary to estimate the influence of exciton effects on the work function of semiconductor nanocrystals.

For quantum-size structures, we calculated the energy levels with regard for the finite height of the



Fig. 3. Work function, forbidden band width, and their sum  $E_g + X$  vs lattice constant for various semiconductors. Dots – tabular data, curves – theoretical results

barrier of the environment and the change of  $m^*$  [11]. In the general form in the approximation of effective mass, we considered the problem of the electron spectrum of a quantum dot with diameter d on the basis of the solution of the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m_e^*(r_e)}\Delta_e - \frac{\hbar^2}{2m_h^*(r_h)}\Delta_h + U(r_e, r_h)\right]\Psi(r_e, r_h) = E\Psi(r_e, r_h)$$
(11)

with the generalized potential  $U(r_e, r_h) = U_{cv}(r) + U_{eh}(r) + U_s(r)$ .

Here,  $U_{cv}(r)$  is the barrier for the V- and C-bands. The coordinate dependences of the effective mass and the potential barrier are introduced as step functions. The energy eigenvalues are obtained by solving the Schrödinger equation for the spherical model of a quantum-size dot [10–13]. Figure 4 illustrates the model of a quantum dot: as the geometric size decreases, the edge of the conduction band shifts to vacuum, and the valence band is deepened.

As for the exciton energies, this problem was solved in [11]. In that model, the electron charge is spread over the volume, whereas a more localized hole oscillates in the field of the electron wave.

The Coulomb interaction potential of an electron and a hole looks as

$$U_{eh}(r) = -\frac{e^2}{4\pi\varepsilon (d)\varepsilon_0} \int \frac{|\Psi(r')|^2}{|r-r'|} d^3r'.$$
(12)



Fig. 4. Effective permittivity vs quantum dot diameter for various surrounding media (1 – hydrated surface, 2 – silicon, 3 – SiO<sub>x</sub>, 4 – SiO<sub>2</sub>, 5 – vacuum). On the right, a model of spherical quantum dot with transient layer is given

To take the image forces  $U_s$  into account, we used the one-dimensional polarization potential which is suitable for estimates in the macroscopic approximation of the effective permittivity:

$$U_s = \frac{1}{n} \sum_{i=1}^{n} \frac{e^2 \left(\frac{\varepsilon_{\rm QD} - \varepsilon(x_i)}{\varepsilon(x_i)}\right)}{4\pi\varepsilon_0 \varepsilon_{\rm QD} \left(\frac{d_{\rm QD}}{2} + x_i\right)}.$$
(13)

By  $d_{\rm QD}$ , we denote the effective diameter of a quantum dot.

In order to take the smooth variation in  $\varepsilon(x_i)$  into account, we approximate it by several (n) rectangular steps. Formula (3) describes the polarization potential created by a one-dimensional rectangular step. The exciton levels are given by the equation [4,5]

$$E_{\rm ex} = \frac{-e^2}{2\pi\varepsilon_{\rm eff}\left(d\right)\varepsilon_0 d}\beta_n + \sqrt{\frac{3\pi\hbar^2 n^2 e^2}{m_{ex}^* d^3\varepsilon_{\rm eff}\left(d\right)\varepsilon_0}}.$$
 (14)

This formula sets the eigenvalues of the potential energy of an oscillator with regard for the motion of an electron and a hole.

In the approximation of effective medium, the formula for the permittivity looks as

$$\varepsilon_{\text{eff}}\left(d\right) = \sum_{i} \varepsilon\left(r_{i}\right) \int_{r_{i}}^{r_{i+1}} r^{2} |\Psi\left(r\right)|^{2} dr$$
(15)

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or in the simpler form

$$\frac{1}{\varepsilon_{\text{eff}}(d)} = \frac{1}{\varepsilon_{\text{Si}}} P_1(d) + \frac{1}{\varepsilon_{\text{SiO}_2}} P_2(d), \qquad (15')$$

where  $P_1(d)$  and  $P_2(d)$  are the weight coefficients of the substances of, respectively, a quantum dot and its environment.

$$\int_{0}^{d/2} r^{2} |\Psi(r)|^{2} dr = P_{1}, \quad \int_{d/2}^{\infty} r^{2} |\Psi(r)|^{2} dr = P_{2}.$$
(15")

It is important to use the normalization condition

$$\int_{0}^{\infty} r^{2} |\Psi x\rangle|^{2} dr = 1.$$
 (15''')

As seen,  $P_1$  and  $P_2$  are the probabilities to find a particle in the quantum dot and outside it. Figure 4 show the dependence of  $\varepsilon_{ef}(d)$  for a Si quantum dot for different  $\varepsilon$  of the environment. We obtain the solution of the Schrödinger equation in the case of the spherical symmetry in the Bessel spherical functions as

$$\Psi_1 = BJ(k,r)$$
 (at the quantum dot), (16)

$$\Psi_2 = AN(\beta, r)$$
 (outside the quantum dot). (16)

Here,

$$\beta = \frac{\sqrt{2m_2^*(U(d) - E)}}{\hbar}, \quad k = \frac{\sqrt{2m_1^*E}}{\hbar}, \tag{17}$$

 $m_{e1}^*$  and  $m_{e2}^*$  are the effective masses of an electron at a quantum dot and outside it. A and B are the constants which define the amplitude of the wave function, and E are the eigenvalues of the ground state.

With regard for the boundary conditions

$$\Psi_1(d/_2) = \Psi_2(d/_2),$$

$$\frac{1}{m_{e,1}^*} \frac{d\Psi_1(d/2)}{dr} = \frac{1}{m_{e,2}^*} \frac{d\Psi_2(d/2)}{dr},$$
(18)

we get the nonalgebraic (transcendental) equation for the determination of the energy parameters of a quantum dot:

$$\frac{\frac{d\beta}{2} - 1}{m_{e,2}^*} = \frac{1 - \frac{dk}{2} \operatorname{ctg}(\frac{kd}{2})}{m_{e,1}^*}.$$
(19)

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Fig. 5. a – Forbidden band widths of quantum-size structures vs quantum dot diameter for various dimensionalities. b – Work functions of quantum-size structures vs quantum dot diameter for various dimensionalities

Its solution gives the allowable levels of kinetic energy for electrons of the quantum structure under study.

An analogous equation can be written also for holes (respectively, with the effective masses  $m_{h1}^*$  and  $m_{h2}^*$ .) In order to determine the constants A and B, it is necessary to use the normalization condition. The obtained energy levels of electrons and holes form the "forbidden zone" of a quantum dot, which can be used for the determination of the work function by formula (9).

In the rough approximation of an infinite barrier, the energy quantization is given by the simple relation

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Fig. 6. a – Forbidden band widths the GaN of quantum-size structures vs quantum dot diameter vs quantum dot diameter for various dimensionalities. b – Work functions of quantum-size structures vs quantum dot diameter for various dimensionalities

 $E = \frac{\pi \hbar^2}{2m^* d^2} \sim \frac{1}{d^2}$ . Since  $m_h \gg m_e$ , the change of the valence band energy on the quantization will be less than that of the conduction band energy.

In Figs. 5–7, we present the values of forbidden band widths and work functions for different dimensions versus the diameter d of a quantum dot for some semiconductors: GaAs, GaN, and Si. It is clear that, in quantum confined structures, the energy parameters vary monotonically with the size d of a structure. A qualitatively similar behavior is demonstrated by bulk structures vs the linear size of an elementary cell L. In all cases, the dependence on d is a monotonic curve decreasing by a power law:  $E_g \sim A/L^n$ , where n is



Fig. 7. Work function and forbidden band width of Si quantumsize structures vs the diameter and quality for of the interface layer. Dots – experimental data

obviously  $1.5\pm 0.5$  (Figs. 4–6). There, we give the data on the electron affinity which is calculated by a relation analogous to (8).

The experimental data for the nanotextured surface of Si are shown in Fig. 7.

It is seen that one size of nanocrystallites corresponds to several experimentally measured energies of optical transitions. This difference is caused by the different conditions of fabrication of specimens: nanostructures with hydrated surface demonstrate the greater energy of the transitions. Nanoclusters with dry oxidized surface have, as a rule, the less energies of optical transitions. We relate it to the influence of parameters of the barrier layer on the level of dimensional quantization [11].

The dependence of the barrier,  $X_0$ , on d were studied experimentally for quantum structures GaN and Si obtained by the method of selective etching [13, 14]. We measured the specimens with the tip radius of a quantum thread ~ 2.5 ±0.5 nm, for which the work function determined by the method of field electron emission from the slope of the Fowler–Nordheim dependences is in the interval  $X_0 = 2.3-2.8$  eV, which is significantly less than the bulk value (3.4 eV). The optical forbidden gap width determined by the photoconductivity spectrum is, on the contrary, significantly greater than the bulk value and is about 4 eV.

For the nanospikes of Si with diameters of 1.5–2.8 nm, we observe experimentally a significant decrease in the work function (down to 3.5 eV) which is essentially less than the bulk work function, whereas the forbidden band width increases respectively to 2.0 eV. Thus, we deal with quantum-size structures. We emphasize also

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Fig. 8. Quantum cathod. Exciton diameter vs quantum dot diameter

good agreement with the above-presented theoretical results according to the formula  $X_0 + E_g = 5.5$  eV -  $\Delta E_{qv}$ ,  $\Delta E_{qv} \leq 0.6$  eV (Fig. 7).

Finally, we note that, for quantum dots of certain substances (with the small effective mass of electrons), the exciton radius can become greater than the size of a quantum dot. This means that the electron leaves the scope of the quantum dot and comes into the environment. That is, we are faced with the case of with negative electric affinity, as it is illustrated by Fig. 8.

#### 4. Conclusions

In the present work, we have analyzed the developed method of calculations of electron affinity (optical work function)  $X_0(L)$  of semiconductor nanocrystals for various lattice constants L which uses the experimentally determined (or calculated) data on the forbidden gap width  $E_g(L)$  and the relation

$$E_g(L) + X_0(L) = 5.5 - \Delta E_{gv}(L) \approx 5.5 \text{ eV}.$$
 (20)

We propose to use this relation also for quantumsize structures, where the relevant parameter will be their size (the diameter d). The agreement of the theoretical results with experimental data was obtained for many bulk crystals of the tetrahedral syngony and for nanocrystals of Si and GaN.

Thus, we have obtained the relation for the energies of quantum states of electrons depending on the geometric sizes of a nanostructure with regard for the

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change of boundary barriers. Earlier, the preliminary calculations were performed for the model of quantum well with infinite barriers or with fixed barriers independent of the well size, and also with arbitrarily given barriers.

In the calculations of band characteristics, we have first used the relations between parameters of the electron structure (the energies of electron levels in a potential well  $E_2$ ) and the work function which were verified for the certain bulk semiconductors.

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#### ВИЗНАЧЕННЯ ЕЛЕКТРОННОЇ СПОРІДНЕНОСТІ (РОБОТИ ВИХОДУ) НАПІВПРОВІДНИКОВИХ НАНОКРИСТАЛІВ

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Резюме

Розроблено метод розрахунку величини електронної спорідненості (оптичної роботи виходу)  $X_0(L)$  напівпровідникових нанокристалів з різними сталими ґратки, який використовує експериментально визнаначені (чи розраховані) значення енергії забороненої зони  $E_g(L)$  та співвідношення  $E_g(L) + X_0(L) = 5,5 - \Delta E_{gv}(L) \approx 5,5$  [еВ]. Це співвідношення пропонується використовувати як для об'ємних, так і для квантоворозмірних структур – в залежності параметрів від діаметра останніх. Проведено перевірку запропонованого співвідношення для напівпровідникових кристалів кубічної модифікації.