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Modeling of Nanometer Scale Physical Objects

Rumyantsev VV*, Fedorov SA, Gumennyk KV and Rybalka AE

State Budget Institution, Galkin Institute for Physics and Engineering, Russian Federation

***Corresponding author:** Rumyantsev VV, State Budget Institution, Galkin Institute for Physics and Engineering, Donetsk, Russian Federation, Email: vladimir.rumyantsev2011@yandex.ru

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Abstract

The paper gives an overall descriptive summary of the properties of nanostructured objects. We dwell in detail on dispersion of polariton excitations in a one-dimensional array of nanoscale cavities with embedded quantum dots as well as on a computer "experiment" which demonstrates the band gap dependence on a nanofilm width.

Keywords: Polariton Excitations; Quantum Dots; Nanostructures; Quantum Size Effect; Energy Band Gap

Introduction

A multitude of macroscopic characteristics of solid bodies (such as density, the Young's modulus, electrical resistivity, magnetization etc.) arise from averaging of corresponding measurable quantities. At micron or nanometer length scales one usually encounters substantially different mechanical, electrical, and optical behaviors [1-5], in particular, nanostructured materials exhibit unusual characteristics and "novel" properties. Let us note that the main physical and chemical properties of materials are defined by corresponding characteristic critical length, which as a rule lie in the nanometer range. For instance, the electro resistivity of a volumetric sample results from the atomic vibration or impurity scattering of conductivity electrons, and characterized by the mean free path of electron is different from that in a nanosample. Another important example of such behavior is given by semiconductor particles whose dimensions are of the order of electron (hole) quantum wavelength of an electron (or hole) in the conductivity band. These are called quantum dots [6] and find broad applications e.g. in fabrication of lasers used for compact disc reading. Electronic structure of a solid state sample strongly depends on the number of dimensions, in which it has nanometer scales. A volumetric nanostructure has a nanoscale size only along *one* of the tree dimensions is called a *quantum well*. Its electronic structure is substantially different from that of nanowires, which have nanoscale sizes along *two* dimensions.

Dependence of electronic properties on object's size results in a substantial difference of optical properties of nanosamples on the corresponding parameters of macroscopic bodies and has an effect on oscillatory spectrum. One of the major problems encountered in fabrication of *nanodevices* deals with the dialectic interaction between the macro- and microscales. For instance, since the eigenfrequency of a rigid rod oscillations increases if its size decreases, for nanoscale dimensions the corresponding frequencies can become as high as 10 THz, whereas the oscillation amplitude lies in the picometer (10^{-15} m) or femtometer (10^{-15} m) range. This should be taken into account when constructing high-frequency sensors capable of detecting minute displacements. Optical deflecting systems used in scanning tunnel microscopes fail to operate if the size of reflector is close to the wavelength of reflected wave and so the diffraction limit comes into play.

Another essential specificity of nanoobjects consists is the role of a *nanostructure surface*. For example almost 10% of atoms of a silicon rod with the length of 100 nm and width of 10 nm are located at the subsurface layer. Such an amount of subsurface atoms considerably affects the sample's mechanical properties (firmness, flexibility etc.).

Quantum Dimensional Effect

Mathematical modeling of the above discussed nanoobjects requires taking into account of their common quality, which is the presence of the so-called quantum dimensional effect. It consists in a drastic change of thermodynamic and kinetic properties of the crystal in the case when at least one of its geometric dimensions is become comparable with de Broglie wavelength. It is connected with energy discretization (quantization) of charge carriers whose motion is limited by potential barriers in one, two or three directions due to a nanometer scale of the sample along a certain axis. In the general case the charge carriers have a discrete spectrum in any volume limited by potential barriers, however the presence of decoherentization results in the broadening of levels and so the energy spectrum has a continuous appearance. In practice the discretization of energy levels of charge carriers can only be observed at a sufficiently small size of the sample at least along one of the directions. Broadening of energy levels due to scattering cannot exceed the distance between them. Dimensions of the domain of limited motion should be much smaller than the mean free path. One needs to obtain small structure sizes, low temperatures along with high mobility of charge carriers. This is attained by a weak scattering and small carrier density resulting in a low Fermi level of the degenerate gas of charge carriers at low temperatures.

Dispersion of Polariton Excitations in a One-dimensional Microcavity Array with Embedded Quantum Dots

To fix the above concepts of nanoobjects let us consider dispersion of polariton excitations in a one-dimensional defect containing two-sublattice array of tunnel coupled nanodimensional cavities (resonators) with embedded atomic nanoclusters (quantum dots) in one (e.g. in the first) of the sublattices. Defects are constituted by cavity position detuning; their concentrations are denoted by C_1 and C_2.

Polari tonic spectrum $\Omega(\mathbf{k})$ of such a system is obtained in the frames of theoretical model outlined in Rumyantsev VV, et al. [7]. It is shown there that diagonalization of the system's averaged Hamiltonian and employment of the virtual crystal approximation along with the nearest neighbor approximation leads to a system of linear homogeneous equations whose solvability condition is the equality to zero of the following determinant:

$$\begin{Vmatrix} \hbar\omega_1^{at} - V_{11}(k) - \hbar\Omega & g_1 & 0 \\ g_1 & \hbar\omega_1^{ph} - \hbar\Omega(k) & -A_{12}(k) \\ 0 & -A_{21}(k) & \hbar\omega_2^{ph} - \hbar\Omega(k) \end{Vmatrix} = 0. \quad (1)$$

Here, $A_{12(21)}$ is the Fourier transform of matrix A_{n1m2}, characterizing an overlap between optical fields of resonators in the $\mathbf{n}1$-th and $\mathbf{m}1$-th lattice sites, and therefore, defining the tunneling transition probability of corresponding electromagnetic excitation, $V_{\mathbf{n}1\mathbf{m}1}$ is the matrix of resonance interaction of quantum dots embedded in the $\mathbf{n}1$-th and $\mathbf{m}1$-th sites, V_{11} is the Fourier transform of this matrix, g_1 describes resonance interaction between a quantum dot and electromagnetic field localized at the same ($\mathbf{n}\alpha$-th) site. The roots of the cubic equation with respect to frequency Ω, resulting from the expansion of determinant (1) were found with the use of program fzero. m from the standard library of the language of technical computing Matlab, based on the Newton iteration algorithm. The modeling values of physical parameters are taken from Rumyantsev VV, et al. [7]. Since the composition of quantum dots remains unchanged parameter has a constant value.

Figure 1 shows the 3d plots of Polariton dispersion law $\Omega_{1,2,3}(k, C_1, C_2)$ (the lower index numerates surface plots from bottom up). The wave number k varies within the first Brillouin zone $-\frac{\pi}{d(C_1, C_2)} < k < \frac{\pi}{d(C_1, C_2)}$ (shaded region in the $(k, C_{1(2)})$-plane in Figure 1).

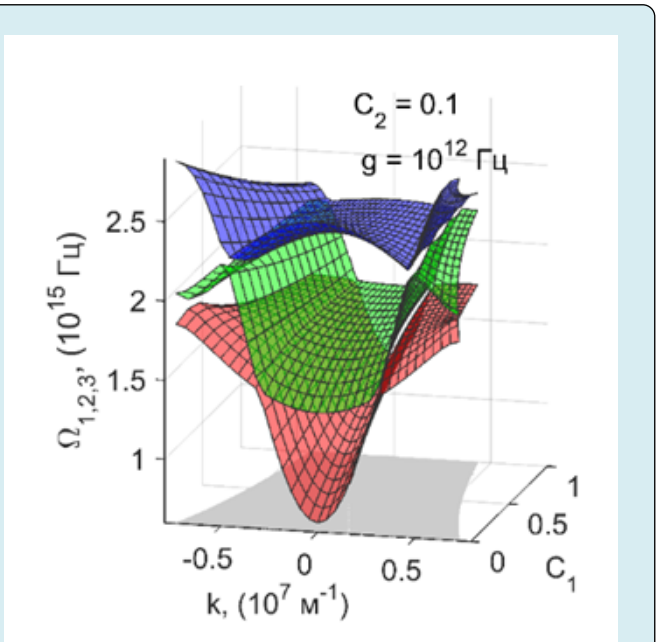

Figure 1: Dependence of Polariton dispersion $\Omega_{1,2,3}(k, C_1, C_2)$ on structural defect for a given value of parameter $g \equiv g_1/\hbar$ of resonance interaction between a quantum dot and electromagnetic field [7].

Examination of the surface plot $\Omega_3(k, C_1, C_2)$ in Figure 1 points to the possibility of existence of Bose-Einstein polariton condensate under a range of values of defect concentrations and both zero non-zero values of wave vector k, which is a non-trivial result.

The Density Functional Theory-based Computer Experiment

The authors of paper [8] show that the band gap E_G of silicon dioxide depends on the bond length Si-O and the bond angle Si-O-Si without taking into account the amount of bonds. There is a distinct correlation between the calculated and experimental [9,10] values of E_G. However there have not been comprehensive studies regarding the dependence of electronic structure parameters of oxides constituting the insulating layer on crystal dimensionality.

At the present time silicon oxide is the key dielectric in silicon devices [11,12], for this reason investigation of electronic properties of a nanocrystal on its composition and the thickness of the ultrathin layer performed in Khachaturova TA, et al. [8] is very interesting. The authors of Khachaturova TA [8] perform a computer "experiment" with the use of the density functional theory and the projector augmented wave method and obtain a number of instructive results regarding electronic structure of a quasi-two-dimensional silicon dioxide crystal whose width is of the order of elementary cell size. Electronic structure of a two-dimensional crystalline structure has been calculated for ultrathin films. It turns out that E_G in SiO_2 films is smaller than that in volumetric crystals and unlike in three-dimensional samples non-monotonically grows with increasing thickness (Figure 2).

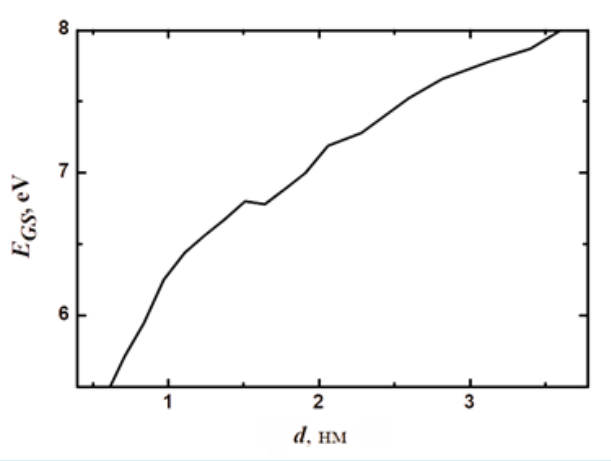

Figure 2: Band gap width dependence in the film thickness for a tetragonal SiO_2 cell type [8].

Conclusion

Nanotechnologies constitute an important part of modern technology paradigm. They permit to fabricate materials, devices and technical systems with peculiar functionalities due to the presence of nanometer scales (e.g. [13]). In addition, they open routes to controllable manipulation of individual atoms and molecules. In practical applications of nanotechnologies one must deal with the fact that the usual macroscopic techniques are often useless at nanoscales, whereas the traditionally neglected microscopic phenomena (interaction between individual atoms, molecules and their aggregates) come to play an important and even decisive role. For this reason an adequate description of nanoobjects requires taking into account the quantum dimensional effect. In the present work this feature of nanoscale systems is reflected in two modeling examples of corresponding physical processes.

Nanotechnologies, unlike the traditional ones, constitute a science-intensive, money-based interdisciplinary endeavor related to physics, chemistry, biology etc. For instance, one of the research areas of modern medicine is directed at possibilities of utilization of nanoobjects for tracing, constructing and altering of human biological systems at a molecular level. To summarize, by all accounts nanotechnologies pertain to high-end endeavors. Another important aspect pertaining to this subject are its socio-economic implications. It can be safely asserted that the results nano-science have a potential to go beyond the limits of purely academic significance and may exert influence on our lifestyle ushering ultimately a new phase of civilizational evolution.

References

1. Lifshitz IM, Kosevich AM (1955) About oscillation of thermodynamic quantities for degenerated Fermi gas at low temperatures. Izv AN SSSR Ser Fiz 19: 395.

2. Sandomirsky VB (1962) On the theory of quantum-size effects in electrical conductivity of semiconductor films. Radiotech Electron 7: 1971-1972.

3. Ogrin F, Lutskii VN, Elinson MI (1966) Observation of quantum size effects in thin bismuth films. ZhETF Pisma Redaktsiiu 3: 114.

4. Tavger BA, Demikhovskii VY (1969) Quantum size effects in semiconducting and semimetallic films. Sov Phys Usp 11(5): 644.

5. Komnik YF, Bukhshtab EI (1968) Observation of the quantum and classical size effects in polycrystalline thin bismuth films. Soviet Journal of Experimental and

Theoretical Physics 27(1): 34-37.

6. Rumyantsev VV, Petrenko AG, Paladyan YA (2022) Quantum nanoparticles: synthesis, properties, applications. Teaching guide. Donetsk National University, Donetsk, pp: 94.

7. Rumyantsev VV, Fedorov SA, Gumennyk KV, Paladyan YA (2022) Specifics of electromagnetic wave propagation through a non-ideal 1D photonic crystal. Physica B: Condensed Matter 629413667.

8. Khachaturova TA, Butko VG, Gusev AA (2022) Electronic structure and properties of two-dimensional silicon dioxide. JETP Lett 115: 41-44.

9. Monaghan S, Hurley PK, Cherkaoui K, Negara MA, Schenk A (2009) Determination of electron effective mass and electron affinity in HfO_2 using MOS and MOSFET structures. Sol St Electron 53(4): 438-444.

10. Govoreanu B, Blomme P, Henson K, Houdt JV, Meyer KD (2003) In Proceedings of the Conference on Simulation of Semiconductor Processes and Devices SISPAD, Boston, USA, IEEE, Computer Society Press, pp: 287.

11. Perevalov TV, Gritsenko VA (2010) Application and electronic structure of high-permittivity dielectrics. Phys Usp 53(6): 561-575.

12. Veksler MI (2015) Increasing the effectiveness of a silicon tunnel MOS-injector of hot electrons using oxides. Technical Physics Letters 41(9): 863-866.

13. Alferov ZI, Aseev AL, Gaponov SV, Kopjev PS, Panov VI (2003) Nanomaterials and nanotechnologies. Nano- and microsystems technology 8: 3-13.