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Elementary particle microstates in sandwich nanostructures

ABSTRACT

This paper analyzes micro-characteristics (single-particle wave functions, the dispersion law of elementary excitations) of sandwich structures. Such structures have exceptional properties and have become current issues in the light of relatively recent discoveries in crystalline structures such as boron nitride-graphene-boron nitride. In our case, structures with a simple cubic lattice are analyzed, but the results can be applied to the structures with monoclinic and triclinic lattices.

Keywords: *Sandwich structure, one-particle wave function, dispersion law of elementary excitations.*

1. INTRODUCTION

The sandwich structure includes the combination of layers (film-structures) of various materials, such as the following types: dielectric-metal-dielectric and metal-dielectric-metal, etc. *The quantum size* and *the surface, i.e. confinement effects* are manifested in these structures. By the combination of different materials and thicknesses of layers, new – desirable properties can be obtained, not possessed by the materials forming the sandwich structure.

Sandwich structures have important practical applications in semiconductors, where combinations of n-p-n and p-n-p semiconductors have characteristics that led to the technological revolution in the second half of the twentieth century. In the 1970s, these structures were extensively investigated in connection to the generation of *high-temperature superconductivity*. It was thought that the effect of the electron–exciton interaction in sandwich structures will lead to a superconductive transition at high temperatures (above 77 K) [1]. A little later (1987), it turned out that the high-temperature (above 77 K) [1]. A little later (1987), it turned out that the high-temperature superconductivity can be realized in the layered structures of copper-oxide compounds [2] with (for now) obscure pairing mechanism of charge carriers in the Cooper pairs.

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Metal sandwich structures have been investigated for more than a decade. Thus, in [3] it is shown that the cellular metals have strength and stiffness attributes that suggest their application as cores for ultra-light panels. The ever-growing interest in these complexes stems from their wide-reaching relevance to catalysis, novel magnetic and optical materials, polymers, molecular recognition, and medical and other applications [4].

In the past decades, numerous researchers have investigated failure strengths and failure mechanisms of sandwich structures [5]. Two-dimensional (2D) nanomaterials, which possess nano-scale dimension in thickness only and infinite length in the plane, have attracted tremendous attention owing to their unique properties and potential applications in the areas of electronics and sensors as well as energy storage and conversion [6]. In particular, recent investigations of graphene, a 2D “aromatic” monolayer of carbon atoms, have demonstrated exceptional physical properties, including ultrahigh electron mobility, ballistic charge carrier transport and other properties.

All above mentioned was our motivation for the theoretical analysis of sandwich structures with a simple cubic lattice. Some cases of complex monoclinic or triclinic structures can be reduced to the equivalent cubic structures [7]. First, we will find an electronic one-particle wave function and the dispersion law depending on the parameters of the structure and the parameters of the boundaries between layers. In further research, we will analyze the thermodynamic properties of these structures.

2. THE MODEL HAMILTONIAN OF SANDWICH STRUCTURE

A simplest model of sandwich synthesized of two ultrathin films of different materials will be analyzed here. It will be assumed that in *z*-direction films have several (not more than 20) layers, while in *xy* planes translational invariance is conserved (schematic presentation of our model is given in Figure 2.1).

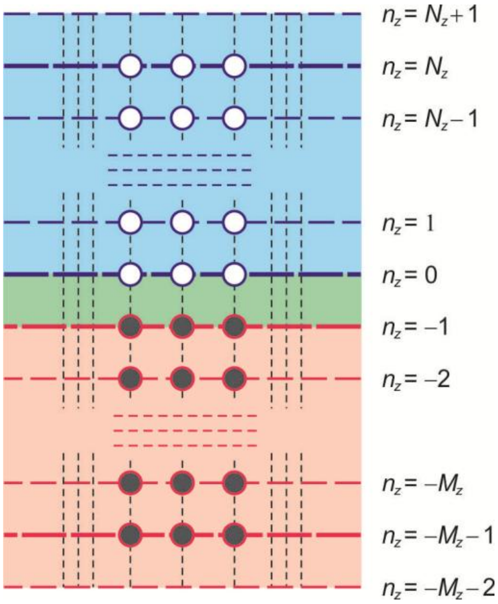

Figure 2.1: Schematic presentations of two coupled films

Slika 2.1: Šematski prikaz dva spregnuta filma

The excitations in described sandwich can be of a very wide spectrum. The stability of excited system depends on characteristics of excitations in each of the films, on boundary conditions, on touching boundary of films and on boundary conditions on external surfaces of sandwich. The stability will be examined by means of free energy of the system.

The Hamiltonian of the system in our research will be of general character, since the types of elementary excitations in film will not be specified. In this general case in the Hamiltonian figure energies of excitations Δ_A and Δ_B of isolated monomers, *P* and *R* for static parts of film's Hamiltonians and *Q* and *S* for transiting (exchange) parts of Hamiltonians. The approximate second quantization method will be applied. It means that Hamiltonians of films are quadratic forms in Bose operators *a* and *b* [8]. The approximation of the nearest neighbors will also be used. It will also be taken that films are cut off from simple cubic structures, which have equal lattice constants d_0. In connection with the last assumption we should point out that in more complicated structures (triclinic or monoclinic), they can be translated into equivalent simple cubic structure. On the Fig. 2.1 the general scheme of layers distribution along *z* axis is given. The presented films contain $N_z + 1$ and $M_z + 1$ planes, respectively, he molecules in planes denoted with $N_z + 1$ and $- M_z - 2$ are absent.

The boundary conditions at the boundary planes n_x, n_y, $\boldsymbol{N_z}$ and n_x, n_y, $-M_z-1$ are:

$$P_{n_x,n_y,N_z;n_x,n_y,N_z+1} = 0 \qquad Q_{n_x,n_y,N_z;n_x,n_y,N_z+1} = 0$$

$$R_{n_x,n_y,-M_z-1;n_x,n_y,-M_z-2} = 0$$

$$S_{n_x,n_y,-M_z-1;n_x,n_y,-M_z-2} = 0 \qquad (2.1)$$

At the planes n_x, n_y, 0 and n_x, n_y,–1 are interacting monomers of different materials (white monomers and black ones). It means that static and transport terms *P*, *Q*, *R* and *S* are not equal to zero, but they can change magnitude and sign. It can be presumed that:

$$P_{n_x,n_y,0;n_x,n_y,-1}, R_{n_x,n_y,0;n_x,n_y,-1} \rightarrow -I_{n_x,n_y,0;n_x,n_y,-1};$$
$$Q_{n_x,n_y,0;n_x,n_y,-1}, S_{n_x,n_y,0;n_x,n_y,-1} \rightarrow -J_{n_x,n_y,0;n_x,n_y,-1}. \qquad (2.2)$$

It should be noted that change of sign in static terms means that the forces between different monomers (white and black) are attractive and that this keeps the sandwich coupled.

Taking into account everything quoted in this section, we can write the Hamiltonian of the sandwich in the following form:

$$H = H_A^{(0)} + H_B^{(0)} + H_{int}, \qquad (2.3)$$

$$H_A^{(0)} = \sum_{n_x,n_y} \Big\{ \sum_{n_z=0}^{N_z} \Delta_A a^{+}_{n_x,n_y,n_z} a_{n_x,n_y,n_z} + 5P\left(a^{+}_{n_x,n_y,0} a_{n_x,n_y,0} + a^{+}_{n_x,n_y,N_z} a_{n_x,n_y,N_z} \right) -$$
$$-Q\ \Big[a^{+}_{n_x,n_y,0} \left(a_{n_x+1,n_y,0} + a_{n_x-1,n_y,0} + a_{n_x,n_y+1,0} + a_{n_x,n_y-1,0} + a_{n_x,n_y,1} \right) +$$
$$+ a^{+}_{n_x,n_y,N_z} \left(a_{n_x+1,n_y,N_z} + a_{n_x-1,n_y,N_z} + a_{n_x,n_y+1,N_z} + a_{n_x,n_y-1,N_z} + a_{n_x,n_y,N_z-1} \right) \Big] + \qquad (2.4)$$

$$+\sum_{n_z=1}^{N_z-1}\Big[6P\,a^{+}_{n_x,n_y,n_z}a_{n_x,n_y,n_z}-Q\,a^{+}_{n_x,n_y,n_z}\Big(a_{n_x+1,n_y,n_z}+a_{n_x-1,n_y,n_z}+$$

$$+a_{n_x,n_y+1,n_z}+a_{n_x,n_y-1,n_z}+a_{n_x,n_y,n_z+1}+a_{n_x,n_y,n_z-1}\Big)\Big]\Big\},$$

$$H_B^{(0)}=\sum_{n_x,n_y}\Big\{\sum_{n_z=-1}^{-M_z}\Delta_B b^{+}_{n_x,n_y,n_z}b_{n_x,n_y,n_z}+5R\Big(b^{+}_{n_x,n_y,-1}b_{n_x,n_y,-1}+b^{+}_{n_x,n_y,-M_z-1}b_{n_x,n_y,-M_z-1}\Big)-$$

$$-S\;\Big[b^{+}_{n_x,n_y,-1}\Big(b_{n_x+1,n_y,-1}+b_{n_x,n_x-1,-1}+b_{n_x,n_y+1,-1}+b_{n_x,n_y-1,-1}+b_{n_x,n_y,-2}\Big)+$$

$$+b^{+}_{n_x,n_y,-M_z-1}\Big(b_{n_x+1,n_y,-M_z-1}+b_{n_x-1,n_y,-M_z-1}+b_{n_x,n_y+1,-M_z-1}+b_{n_x,n_y-1,-M_z-1}+b_{n_x,n_y,-M_z}\Big)\Big]+$$

$$+\sum_{n_z=-2}^{-M_z}\Big[6R\,b^{+}_{n_x,n_y,n_z}b_{n_x,n_y,n_z}-S\,b^{+}_{n_x,n_y,n_z}\Big(b_{n_x+1,n_y,n_z}+b_{n_x-1,n_y,n_z}+\qquad(2.5)$$

$$+b_{n_x,n_y+1,n_z}+b_{n_x,n_y-1,n_z}+b_{n_x,n_y,n_z+1}+b_{n_x,n_y,n_z-1}\Big)\Big]\Big\},$$

$$H_{int}=-\sum_{n_x,n_y}\Big[I\Big(a^{+}_{n_x,n_y,0}a_{n_x,n_y,0}+b^{+}_{n_x,n_y,-1}b_{n_x,n_y,-1}\Big)+J\Big(a^{+}_{n_x,n_y,0}b_{n_x,n_y,-1}+b^{+}_{n_x,n_y,-1}a_{n_x,n_y,0}\Big)\Big]\;.(2.6)$$

3. ONE-PARTICLE STATES OF SANDWICH STRUCTURE

The analysis of properties of the sandwich, which Hamiltonian is given by (2.3), will be done in terms of one-particle wave functions. In the analysis of one-particle wave function of the sandwich, we shall start with the well-known wave function of an ideal cubic structure and then we shall look for the wave function of films making the sandwich.

This means that in the first stage we shall look for wave functions of the parts of the sandwich. The part of the sandwich is a broken symmetry structure, containing white points, with boundary conditions:

$$P_{n_x,n_y,N_z;n_x,n_y,N_z+1}=0;\qquad P_{n_x,n_y,0;n_x,n_y,-1}=0;$$
$$Q_{n_x,n_y,N_z;n_x,n_y,N_z+1}=0;\qquad Q_{n_x,n_y,0;n_x,n_y,-1}=0.\qquad(3.1a)$$

In the part of the sandwich, containing black points, boundary conditions are:

$$R_{n_x,n_y,-M_z-1;n_x,n_y,-M_z-2}=0;\qquad R_{n_x,n_y,0;n_x,n_y,-1}=0;$$
$$S_{n_x,n_y,-M_z-1;n_x,n_y,-M_z-2}=0;\qquad S_{n_x,n_y,0;n_x,n_y,-1}=0.$$
(3.1b)

The wave function of the part of the sandwich corresponding to white point (upper film in the Fig. 2.1) will be taken in the form:

$$\Big|\Psi^{(A)}_{k_x.k_y,\nu}\Big\rangle=\frac{1}{\sqrt{N_xN_y\left(N_z+1\right)}}\sum_{n_x,n_y}\sum_{n_z=0}^{N_z}A_{n_x,n_y,n_z;k_x,k_y,\nu}a^{+}_{n_x,n_y,n_z}\left|0\right\rangle.\qquad(3.2)$$

The coefficients A will be taken as

$$A_{n_x,n_y,n_z;k_x,k_y,\nu}=\alpha_{n_z,\nu}\,e^{id_0k_xn_x+id_0k_yn_y},\qquad(3.3)$$

where coefficients

$$\alpha_{n_z,\nu}=sin\left(n_z+1\right)\theta_\nu-\frac{P}{Q}sin\,n_z\theta_\nu,\qquad(3.4)$$

with the condition:

$$sin\left(N_z+2\right)\theta_\nu-2\frac{P}{Q}sin\left(N_z+1\right)\theta_\nu+\left(\frac{P}{Q}\right)^2sin\,N_z\theta_\nu=0\qquad(3.5)$$

satisfy the system of homogenous equations:

$$\sum_{\nu} \left(2Q\cos\theta_{\nu} + \rho_A\right)\alpha_{n_z,\nu} = 0 \qquad n_z = 0,1,2,...,N_z \tag{3.6}$$

where

$$\rho_A \equiv \rho_A\left(k_x,k_y\right) = E - \Delta_A - 6P + 2Q\left(\cos d_0k_x + \cos d_0k_y\right). \tag{3.7}$$

The system of homogenous equations for $\alpha_{nz,\nu}$ is satisfied only for: $2Q\cos\theta_\nu + \rho_A = 0$, and this gives the energies of excitations created by operators

$$E_A\left(k_x,k_y,\nu\right) = \Delta_A + 6P - 2Q\left(\cos d_0k_x + \cos d_0k_y + \cos\theta_{\nu}\right); \quad \nu = 0,1,2,...,N_z+1 \tag{3.8}$$

The wave function of the second part of the sandwich corresponding to black point can be found analogously as $\left|\Psi_{k_x.k_y,\nu}(A)\right\rangle$. Therefore, derivation will be omitted and only the final result will be quoted:

$$\left|\Psi^{(B)}_{k_x.k_y,\mu}\right\rangle = \frac{1}{\sqrt{M_xM_y\left(M_z+1\right)}}\sum_{n_x,n_y}\sum_{n_z=-1}^{-M_z-1} B_{n_x,n_y,n_z;k_x,k_y,\mu}\, b^{+}_{n_x,n_y,n_z}\left|0\right\rangle \tag{3.9}$$

$$B_{n_x,n_y,n_z;k_x,k_y,\mu} = \beta_{n_z,\mu}\, e^{id_0k_xn_x + id_0k_yn_y}; \qquad \beta_{n_z,\mu} = \sin n_z\varphi_\mu - \frac{R}{S}\sin\left(n_z+1\right)\varphi_\mu \tag{3.10}$$

$$\sin\left(M_z+2\right)\varphi_\mu - 2\frac{R}{S}\sin\left(M_z+1\right)\varphi_\mu + \left(\frac{R}{S}\right)^2\sin M_z\,\varphi_\mu = 0.$$

$$\sum_{\nu}\left(2Q\cos\varphi_\mu + \rho_{\mathrm{B}}\right)\beta_{n_z,\mu} = 0; \quad n_z = -1,2,...,-M_z-1 \tag{3.11}$$

$$\rho_B \equiv \rho_B\left(k_x,k_y\right) = E - \Delta_B - 6R + 2S\left(\cos d_0k_x + \cos d_0k_y\right) \tag{3.12}$$

From (3.11) follows: $2S\cos\varphi_\nu + \rho_{\mathrm{B}} = 0$, wherefrom energies of excitations in the second part of the sandwich are:

$$E_B\left(k_x,k_y,\mu\right) = \Delta_B + 6R - 2S\left(\cos d_0k_x + \cos d_0k_y + \cos\varphi_\mu\right); \quad \mu = 1,2,...,M_z+1 \tag{3.13}$$

The wave function (3.2) and (3.9) are determined but they are not normalized. Their normalization is necessary for further applications. Using the normalization procedure of the ideal structure [9], the normalized wave functions that describe the behavior of excitations separately in part A (white molecules) and in part B (black molecules) of our sandwich-model are:

$$\left|\Psi^{(A)}_{k_x.k_y,\nu}\right\rangle_N = \frac{1}{\sqrt{N_xN_y\,\sigma_\nu}}\sum_{n_x,n_y}\sum_{n_z=0}^{N_z} e^{id_0n_xk_x + id_0n_yk_y}\alpha_{n_z,\nu}\, a^{+}_{n_x,n_y,n_z}\left|0\right\rangle; \quad \sigma_\nu = \sum_{n_z=0}^{N_z}\alpha^2_{n_z,\nu} \tag{3.14}$$

$$\left|\Psi^{(B)}_{k_x,k_y,\mu}\right\rangle_N = \frac{1}{\sqrt{N_xN_y\,\eta_\mu}}\sum_{n_x.n_y}\sum_{\mu=1}^{M_z+1} e^{id_0n_xk_x + id_0n_yk_y}\beta_{n_z,\mu}\, b^{+}_{n_x.n_y,n_z}\left|0\right\rangle; \quad \eta_\mu = \sum_{n_z=-1}^{-M_z-1}\beta^2_{n_z,\mu}. \tag{3.15}$$

Having normalized functions of parts of the sandwich as the functions of zero order approximations, we can find expressions for energies of elementary excitations in the sandwich and wave functions in the first order approximation by means of standard formulae for stationary perturbations.

The analysis of the simplest sandwich structure: two coupled films – can be done by using the functions (3.14) and (3.15). However, this is connected to specific physical problems, i.e. material/composition and dimensions of the sample.

On the other hand, regardless of this, several key results can be seen from the results obtained. As the main finding, we would like to emphasize that the quantum effects can be seen from the explicit form of the formulas for the wave function of the system (3.14) and (3.15) – e.g. when the formulae for possible (discrete) values of *z*-components of quasi-impulses [10]:

$$k_z^{(A)} = \frac{\pi \nu}{N_z + 2}; \quad \nu = 1, 2, 3, \dots, N_z+1;$$

$$k_z^{(B)} = \frac{\pi \mu}{M_z + 2}; \quad \mu = 1,2,3, \dots N_z+1$$

are combined with the allowed (discrete) energies of the system of elementary excitations (3.8) and (3.13). This means that all the essential concomitants of nanostructures are present in sandwich structures: quantum size effect without confinement effects. These effects are consequences of the dimensions and specific form/composition of the sandwich structure, and provide for their fundamentally different macroscopic properties (similar to the other nanostructures) in relation to the corresponding bulk samples.

4. CONCLUSION

This paper analyzes the micro characteristics of a sandwich structure consisting of the crystalline films of different materials, as well as a semi-infinite structure consisting of a film and a substrate. The corresponding Hamiltonian system of general type was used for the analysis, and the type of elementary excitation s that occur in the system has not been specified. The one-particle wave function and the dispersion law of elementary excitations were found as quantities that contain micro-characteristics of the system. These quantities are expressed through elementary cell constants, the number of atomic layers in the films (through the film thickness) and the quantities defining the elementary excitations of the isolated monomers as well as the quantities defining the exchange energy in the Hamiltonian.

These results are of general importance. By finding empirical data for the corresponding concrete structures, it is easy to find values for required sizes. All this will enable us to find relevant macroscopic thermo- or electro-dynamics, optical and other physical quantities/properties of these structures in our future research [11].

In the paper was solved problem of broken symmetry parts of sandwich, only. The interaction between parts of sandwich was not taken into account now. Using theory of stationary perturbation, we can determine the corrections to the energy due to this interaction. This will be the subject of another paper.

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5. REFERENCES

[1] V.L.Ginzburg (1976) High-temperature superconductivity-dream or reality? Sov. Phys. Usp., 19**,** 174–179.

[2] J.P.Šetrajčić (1998) Superconductivity and Fullerenes, Materials Sci. Forum, 282-283, 71-82.

[3] M.F.Ashby, A.G.Evans, N.A.Fleck, G.L. Gibson, J.W. Hutchinson, H.G.N.Wadley (2000) Metal Foams: a Design Guide, Butterworth Heinemann, London 2000.

[4] N.J. Long (1998) Metallocenes; Blackwell Science, Oxford 1998.

[5] D.W. Sleight, J.T. Wang (1995) Buckling Analysis of Debonded Sandwich Panel under Compression, Hampton, VA: NASA LaRC 1995.

[6] E. Antolini (2009) Palladium in fuel cell catalysis, Energy Environ*. Sci*., **2**, 915–931.

[7] V.D.Sajfert, S.K.Jaćimovski, D.Popov, B.S.Tošić (2007) Statistical and Dynamical Equivalence of Different Elementary Cells, J. Comput. Theor. Nanosci*.*, **4**(3), 619-626.

[8] P.A.M.Dirac (1958) Principles of Quantum mechanics, Oxford UP, Oxford 1958.

[9] V.D.Sajfert, B.S.Tošić (2010) The Research Nanoscience Progress, J. Comput. Theor. Nanosci*.*, **7**/1, 15-84.

[10] J.P.Šetrajčić, D.Lj.Mirjanić, V.D.Sajfert, B.S.Tošić (1992) Perturbation Method in the Analysis of Thin Deformed Films and the Possible Applications, Physica A, **190**, 363-374.

[11] V.D.Sajfert, J.P.Šetrajčić (2022) Application of Green's functions and difference equations in theoretical analyses of nanostructures, In: Series on the foundations of natural science and technology, Vol. 15 Topics in nanoscience, Part I: Basic views, complex nanosystems: Typical results and future, Ed. W. Schommers; World Scientific, Singapore; 7, 311-412.

IZVOD

MIKROSTANJA ELEMENTARNIH ČESTICA U SENDVIČ NANOSTRUKTURAMA

U ovom radu se analiziraju mikrokarakteristike (jednočestične talasne funkcije, zakon disperzije elementarnih pobuđenja) sendvič struktura. Takve strukture imaju izuzetna svojstva i postale su aktuelna u svetlu relativno nedavnih otkrića u kristalnim strukturama kao što su bor nitrid-grafen-bor nitrid. U našem slučaju se analiziraju strukture sa jednostavnom kubičnom rešetkom, ali se rezultati mogu primeniti na strukture sa monokliničkim i trikliničkim rešetkama.

Ključne reči: *Sendvič strukture, jednočestična talasna funkcija, zakon disperzije elementarnih ekscitacija.*

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