ANNALS of Faculty Engineering Hunedoara – International Journal of Engineering
Tome XX [2022] | Fascicule 4 [November]

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MICROSTATES OF ELEMENTARY EXCITATIONS IN SANDWICH NANO–STRUCTURES

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Abstract: In this paper we have analysed some specific properties of nanostructures that build form of the sandwich. Those properties represent micro–characteristics expressed through the single–particle wave functions and the dispersion law of elementary excitations. Sandwich structures have some exceptional properties and they came to focus of recent discoveries, especially in structures such as boron nitride–graphene–boron nitride. We have analysed and narrowed our research to the structures with a simple cubic lattice, but the obtained results can be applied to the structures with monoclinic and triclinic lattices.
Keywords: Sandwich structures, specific properties of nanostructures

1. INTRODUCTION

The sandwich nano–structure includes the combination of nano–layers (ultrathin film–structures) of various materials, such as the following types: dielectric–metal–dielectric and metal–dielectric–metal, etc. Such structures show confinement effects – the effects caused by the quantum size of these structures and interaction between the surface and surrounding matter (or vacuum). One can obtain new – desirable properties by the combination of different materials and thicknesses of layers. The same properties could not be obtain with the solely materials, but only when they form the structure of the sandwich.

Sandwich nano–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 nano–structures will lead to a superconductive transition at high temperatures (over 77 K) [1]. A little later (1987), it turned out that the high–temperature superconductivity can be realized in the layered nano–structures of copper–oxide compounds [2] with (for now) obscure pairing mechanism of charge carriers in the Cooper pairs.

Metal sandwich nano–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, medical and other applications [4].

In the past decades, numerous researchers have investigated failure strengths and failure mechanisms of sandwich nano–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 values of the 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 NANO–STRUCTURE

We have proposed a simple model of sandwich synthesized of two ultrathin films made of different materials. Let us assume 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 1).

The excitations in described sandwich could have very wide spectrum. The stability of excited system depends on characteristics of excitations in each of the films and on boundary conditions. When we analyze boundary conditions – we have one boundary layer between films and various boundary conditions on external surfaces of sandwich. The stability is examined trough the free energy of the system.

The Hamiltonian of the system in our research have general character, since the types of elementary excitations in film is not exactly 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.

Next, we have applied the approximate second quantization method. It means that Hamiltonians of films have quadratic forms in Bose operators a and b [8]. In addition, we have used the approximation of the nearest neighbors and assumed that the films are cut off from simple cubic structures, which have equal lattice constants d_0. The reason for the last assumption is the fact that more complicated structures, such as triclinic or monoclinic ones, they can be translated into equivalent simple cubic structure. On the Fig. 2.1 is shown the general scheme of layers distribution along z–axis. The presented films contain N_z+1 and M_z+1 planes, respectively, where the molecules in planes denoted with N_z+1 and $-M_z-2$ are absent.

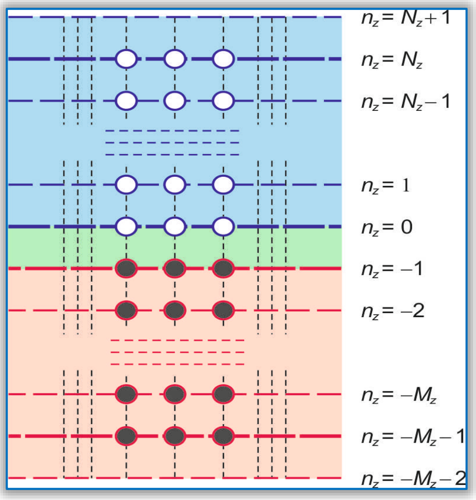

Figure 1. Schematic presentations of two coupled films

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

$$P_{n_x,n_y,N_z;n_x,n_y,N_z+1}=0; \qquad Q_{n_x,n_y,N_z;n_x,n_y,N_z+1}=0;$$
$$R_{n_x,n_y,-M_z-1;n_x,n_y,-M_z-2}=0; \qquad S_{n_x,n_y,-M_z-1;n_x,n_y,-M_z-2}=0. \tag{2.1}$$

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:

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

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 above, we can write the Hamiltonian of the sandwich in the following form:

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

$$\begin{aligned} H_A^{(0)} = \sum_{n_x,n_y} \Bigg\{ & \sum_{n_z=0}^{N_z} \Delta_A a^+_{n_x,n_y,n_z} a_{n_x,n_y,n_z} + 5P\left(a^+_{n_x,n_y,0} a_{n_x,n_y,0} + a^+_{n_x,n_y,N_z} a_{n_x,n_y,N_z}\right) - \\ & -Q\Big[a^+_{n_x,n_y,0}\left(a_{n_x+1,n_y,0} + a_{n_x-1,n_y,0} + a_{n_x,n_y+1,0} + a_{n_x,n_y-1,0} + a_{n_x,n_y,1}\right) + \\ & + a^+_{n_x,n_y,N_z}\left(a_{n_x+1,n_y,N_z} + a_{n_x-1,n_y,N_z} + a_{n_x,n_y+1,N_z} + a_{n_x,n_y-1,N_z} + a_{n_x,n_y,N_z-1}\right)\Big] + \\ + \sum_{n_z=1}^{N_z-1}\Big[6P\, a^+_{n_x,n_y,n_z} a_{n_x,n_y,n_z} & - Q\, a^+_{n_x,n_y,n_z}\left(a_{n_x+1,n_y,n_z} + a_{n_x-1,n_y,n_z} + + a_{n_x,n_y+1,n_z} + a_{n_x,n_y-1,n_z} + a_{n_x,n_y,n_z+1} + a_{n_x,n_y,n_z-1}\right)\Big]\Bigg\}, \end{aligned} \tag{2.4}$$

$$\begin{aligned} H_B^{(0)} = \sum_{n_x,n_y} \Bigg\{ & \sum_{n_z=-1}^{-M_z} \Delta_B b^+_{n_x,n_y,n_z} b_{n_x,n_y,n_z} + 5R\left(b^+_{n_x,n_y,-1} b_{n_x,n_y,-1} + b^+_{n_x,n_y,-M_z-1} b_{n_x,n_y,-M_z-1}\right) - \\ & -S\Big[b^+_{n_x,n_y,-1}\left(b_{n_x+1,n_y,-1} + b_{n_x,n_x-1,-1} + b_{n_x,n_y+1,-1} + b_{n_x,n_y-1,-1} + b_{n_x,n_y,-2}\right) + \\ & + b^+_{n_x,n_y,-M_z-1}\left(b_{n_x+1,n_y,-M_z-1} + b_{n_x-1,n_y,-M_z-1} + b_{n_x,n_y+1,-M_z-1} + b_{n_x,n_y-1,-M_z-1} + b_{n_x,n_y,-M_z}\right)\Big] + \\ + \sum_{n_z=-2}^{-M_z}\Big[6R\, b^+_{n_x,n_y,n_z} b_{n_x,n_y,n_z} & - S\, b^+_{n_x,n_y,n_z}\left(b_{n_x+1,n_y,n_z} + b_{n_x-1,n_y,n_z} + b_{n_x,n_y+1,n_z} + b_{n_x,n_y-1,n_z} + b_{n_x,n_y,n_z+1} + b_{n_x,n_y,n_z-1}\right)\Big]\Bigg\} \end{aligned} \tag{2.5}$$

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

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 in the sandwich, we shall start with the well–known wave function of an ideal cubic structure and then look for the wave function of films, from which the structure of sandwich is made of.

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 structure with broken symmetry (white molecules in Fig.1), with boundary conditions:

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

In the part of the sandwich (black molecules in Fig.2.1), boundary conditions are:

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

The wave function of the part of the sandwich corresponding to white point have the form:

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

The coefficients A are:

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

where coefficients

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

with the condition:

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

satisfy the system of homogenous equations:

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

where

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

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

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

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 here is omitted and the final result is:

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

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

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

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

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

From (3.11) follows: $2S\cos\varphi_\nu+\rho_B=0$, where from energies of excitations in the second part of the sandwich are:

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

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:

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

$$\left|\Psi^{(B)}_{k_x,k_y,\mu}\right\rangle_N = \frac{1}{\sqrt{N_x N_y \eta_\mu}} \sum_{n_x.n_y} \sum_{\mu=1}^{M_z+1} e^{id_0 n_x k_x + id_0 n_y k_y} \beta_{n_z,\mu} b^{+}_{n_x.n_y,n_z} \left|0\right\rangle; \quad \eta_\mu = \sum_{n_z=-1}^{-M_z-1} \beta^2_{n_z,\mu}. \qquad (3.15)$$

With the zero order approximations of normalized functions, one can derive expressions for energies of elementary excitations in the sandwich and wave functions in the first order approximation using standard formulae for stationary perturbations.

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

From the obtained results one can obtain several key results. Among them, we want to emphasize that the quantum effects, that can be seen in the explicit form of the formulas for the wave function of the system (3.14) and (3.15) – e.g. from where the formulae for possible (discrete) values of z–components of quasi–impulses [10]:

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

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. CONCLUSIONS

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 excitations that occur in the system has not been specified. The one–particle wave function and the dispersion law of elementary excitations were found as terms that contain micro–characteristics of the system. These terms are expressed through the elementary cell constants, the number of atomic layers in the films (through the film thickness) and the terms defining the elementary excitations of the isolated monomers, as well as the terms defining the exchange energy in the Hamiltonian.

All obtained 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. In the paper was solved problem of broken symmetry in parts of sandwich only. The interaction between these parts of sandwich was not taken into account, for now. Using theory of stationary perturbation, we can determine the corrections to the energy due to this interaction and that will be the subject of further research.

Acknowledgements: The authors of this paper owe the greatest gratitude to their teacher, mentor and friend, unfortunately recently deceased, Academician, Prof. Dr. Bratislav S. Tošić. His proper and quality suggestions had a crucial impact on the value and importance of this work. This work was partially supported by the Ministry of Scientific and Technological Development, Higher Education and Information Society (Grants: 19.032/961–36/19 and 19.032/961–42/19) of Republic of Srpska Government.

Note: This paper was presented at International Conference on Applied Sciences – ICAS2022, organized by University Politehnica Timisoara, Faculty of Engineering Hunedoara (ROMANIA) and University of Banja Luka, Faculty of Mechanical Engineering Banja Luka (BOSNIA & HERZEGOVINA), in May 25–28, 2022, in Banja Luka (BOSNIA & HERZEGOVINA).

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ISSN 1584 – 2665 (printed version); ISSN 2601 – 2332 (online); ISSN–L 1584 – 2665