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THE SELF- COORDINATED COMPUTATION OF ELECTRONIC POWER SPECTRUM AND WAVE FUNCTION IN CRYSTALS WITH TYPE STRUCTURE TO DIAMOND

Keywords: crystals, structure, power spectrum, wave function

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The calculations of self-coordinated power spectrum in the basic high symmetrical зБ, ΓL and ΓX directions are stated in this article. Because the germanium has a lesser width of forbidden zone in comparison by silicon, that approximates it to metals, then influence of correlation effects becomes prettily perceptible. That's why attached to E(κ) calculations of germanium the correlation amendments are included into crystalline potential. The analysis of results calculations shows, that an increasing of base length to 331 ПХ brings to energy values stabilization, which are close to experimental.

1. INTRODUCTION

One of the basic problems of quantum theory of solid there is a computation of electronic power spectrum and wave functions, which determine a lot of quasi-conductors properties. Self-particle own energies and wave functions find from determinations of system of linear homogeneous equations in flat-waved conception:

$$\sum_{\vec{G}}\left[\left(\left(\vec{k}+\vec{G}\right)^2 - E_{n,\vec{k}}\right)\delta_{i,j} + W_{i,j}(\vec{G})\right] a_{n,\vec{k}}(\vec{G}) = 0 \qquad (1)$$

In system (1): $E_{n,\vec{k}}$ - unknown power spectrum, $\vec{k}$ - vector from first Briljuen zone, $\vec{G}$ - vector of reverse lattice and $a_{n/\vec{k}}(\vec{G})$ - are the unknown coefficients of wave vector analysis.

The quasi - potential $w(\vec{r})$ will give as sum $w_i(\vec{r})$ of local Beritonchini-Meloni quasi - potential [1] and a screening items: potentials of coulomb $V_H(\vec{r})$ and exchange - correlation interaction [2]:

$$w(\vec{r}) = w_i(\vec{r}) + V_H(\vec{r}) + V_{X,C}(\vec{r}) \qquad (2)$$

2. EXPERIMENTAL PART

As the coulomb and exchange-correlation potentials depend on distribution of electronic density in crystal, then search task of crystal power spectrum necessary to determine as self-coordinated one. The scheme of our computations is such. The electronic density builds on an atomic wave functions on the zero iterations [3]. The coulomb potential calculates by the Poisson equation, being based on atomic electronic density. The exchange – correlation potential calculates in X_α - approximation. A potential (2) got in such approach puts into secular equation (1). The solutions of this equation will be the wave functions $\Psi_{n,\vec{k}}(\vec{r})$, which have periodicity crystalline lattice properties. By following step of self - coordination is a construction of electronic crystal density $\rho(\vec{r})$ on Bloh wave functions and correction of coulomb and exchange - correlation potentials.

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If found, then matrix element of coulomb potential is:

$$V_H(\vec{r}) = \frac{8\pi\rho(q)}{\Omega_o q^2} . \tag{3}$$

As the electronic density $\rho(q)$ enters into exchange – correlation potential with 1/3 power, then attached to computations of matrix elements $V_{X,C}(\vec{r})$ arises the problem of finding an integral of type [4]:

$$I(q) = \frac{1}{\Omega}\int_x\int_y\int_z \varphi(x,y,z)^{1/3} e^{-i(q_x x + q_y y + q_z z)} dxdydz , \tag{4}$$

This problem can be determined by the numeral methods. The function $\exp(-iqr)$, which enters under integral in (4), brings the considerable oscillations into conduct of underintegral function at $|q|$ grand meanings. Such problem of quickly oscillated functions integration can be calculated, if the function $\exp(-iqr)$ will single out as balance factor [5]. The quadrature formula for chance function of three variable f(x,y,z) will be written:

$$\int_{a_1}^{b_1}\int_{a_2}^{b_2}\int_{a_3}^{b_3} f(x,y,z) e^{-i(q_x x + q_y y + q_z z)} dxdydz = S_n(q) , \tag{5}$$

$$S_n(q) \approx \frac{b_1 - a_1}{2}\frac{b_2 - a_2}{2}\frac{b_3 - a_3}{2}\exp\left\langle -iq_x \frac{b_1 + a_1}{2}\right\rangle \exp\left\langle -iq_y \frac{b_2 + a_2}{2}\right\rangle *$$
$$* \exp\left\langle -iq_z \frac{b_3 + a_3}{2}\right\rangle \sum_i\sum_j\sum_k c_{i,j,k} D_{i-1}(p_x) D_{j-1}(p_y) D_{k-1}(p_z) \tag{6}$$

where $D_{i-1}, D_{j-1}, D_{k-1}$ - approximation coefficients of electronic density in straight space.

An interpolation formula for single scale case has appearance is:

$$f(x) = \sum_{i=1}^{n} c_i T_{i-1}(x) - 0.5c_1 ,$$

where

$$c_i = 2/n \sum_{j=1}^{n} f\left[\cos\frac{\pi(j-0,5)}{n}\right]\cos\frac{\pi(i-1)(j-0,5)}{n} \tag{7}$$

The Chebyshev polynomial $T_n(x)$ for $n \geq 0$, is calculated by recurrent equation:

$$T_o(x) = 1;\ T_1(x) = x;$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) . \tag{8}$$

A calculations of power silicon spectrums will self-coordinated by directed algorithm of coulomb and exchange-correlation potentials computation.

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3. RESULTS AND DISCUSSION

The analysis results given in table 1 shows, that the satisfactory transitions sizes: $\Gamma_{25}' \rightarrow \Gamma_{15}$, $\Gamma_1(1) \rightarrow \Gamma_{25}'$, $\Gamma_{25}' \rightarrow X_4$, $\Gamma_{25}' \rightarrow L_{2'}(l)$, $\Gamma_{25}' \rightarrow L_1(l)$, $\Gamma_{25}' \rightarrow L_3$', et al., are after first iteration. A size of zone forbidden width E_{gap} is inhibited from the understated but conveniences for calculations on base of local density functional [6, 7].

An increasing of base length of secular task leads to results stabilization, which are close to experimental for many transitions (table 1).

Table 1

The self-coordinated own energy values into eV in Γ, X, L points for silicon

Level	The basis size			
	137*137	229*229	331*331	The experiment [7]
E_{gap}	0.40	0.43	0.44	1.17
$\Gamma_1(1)$	-12.39	-12.30	-12.28	-12.5±0.5
Γ_{25}'	0.00	0.00	0.00	0.00
Γ_{15}	2.81	2.91	3.01	3.4
Γ_2'	6.49	5.79	5.54	4.2
$\Gamma_1(2)$	8. 11	7.55	7.48	-
Γ_{12}'	8.44	9.04	9.15	-
$X_1(1)$	-7.92	-7.87	-7.88	-
X_4	-3.24	-3.19	-3.14	-2.9±0.2
$X_1(2)$	0.54	0.55	0.57	1.3
X_3	10.65	10.68	10.73	-
L_2'	-10.288	-9.71	-9.73	-9.4±0.4
$L_1(1)$	-7.539	-7.39	-7.34	-6.7±0.2
L_3'	-1.375	-1.23	-1.24	-1.2±0.2
$L_1(2)$	1.712	2.33	2.24	2.1±0.15
L_3	3.580	3.38	3.46	4.15±0.1
$L_2'(2)$	7.521	7.04	7.02	-

The increasing of base length does not influence substantively on general curves motion of zone spectrum.

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4. CONCLUSIONS

Comparing the results of silicon zones calculations there can be deduced, that it is possible to be accorded kind coordination of theory and experiment for some basic between zone transitions. But coordination for all of transitions was not reached yet.

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A STUDY OF THE FEASIBILITY OF USING LOW COST THICK FILM TRACKS IN THE LOWER PART OF THE MICROWAVE SPECTRUM

Key words: Thick film conductors, microwave properties, microwave measurements, quality control

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Conventionally it is accepted that conductors for low microwave applications should meet a range of electrical and topographic criteria in order to perform correctly. These include a minimum thickness due to skin effects, smooth track and substrate surfaces and rectilinear geometry. The metal must also be very dense and uniform and have the highest possible electrical conductivity. As a result, photolithographically defined gold tracks are preferred and may be made in either thick or thin film.

The paper briefly reviews these requirements and presents results for both idealised and real track materials. Aluminium, gold, copper and silver, in order of increasing conductivity are candidate materials. In practice, only gold and silver are found in most industrial applications. Losses in the best real tracks compare very well with the theoretical predictions.

However, the penalty is cost and, despite some disadvantages, silver is a viable alternative to gold. Standard thick film techniques produce inferior definition, density and surface roughness, but

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