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Gdańsk

Symmetry-Adapted Wave Functions for Crystal Surface*

The character tables and the symmetry-adapted wave functions have been determined in a systematic way for non-symmorphic two-dimensional space group for $x-y$ surface of white tin lattice. Actual calculations in the present work have been confined to four wave vectors of the two-dimensional Brillouin zone.

These functions may be used for calculations of the electronic properties of thin or thick films by means of multiple-scattering method.

Nomenclature

SUC	– surface unit cell,	$\vec{k}^s$	– wave vector,
AS	– atomic segment,	E, I	– identity and inversion operators,
$\vec{\tau}$	– non-primitive translation,	C, σ	– rotation and reflection operators,
G^s	– two-dimensional space group,	$\psi(\vec{r})$	– wave function,
BZ	– Brillouin zone,	P^p_{mn}, P^p	– projection operators.

1. Introduction

In the band structure calculations, concerning both the bulk and the surface of crystals, it is necessary to know wave functions transforming according to the irreducible representation of the corresponding space group. In this work we are interested in the construction of such functions for white tin crystal surface which is treated within a slab geometry.

The preponderance of works analysing surface electronic structures are based on a slab geometry rather than on a semi-infinite geometry.

In the latter case the symmetry is reduced, because there is no reflection symmetry in the plane $z=0$ (Fig. 2), and in some cases there is no inversion symmetry.

The value of this simple model is that calculations of surface properties can be performed for simple metals, semiconductors, transition metals and for surface conditions

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such as clean, reconstructed, relaxed and chemisorbed systems [1]. Its weakness lies in the fact that the computational effort grows considerably with the increasing number of layers.

In considering surface properties of white tin we assume that the surface in question is a natural face of the bulk crystal. For labelling of the symmetry operations in this paper the Schoenflies notation is being used. We shall follow the notation of Cracknell in labelling the two-dimensional point and space groups.

2. Group analysis of the surface region

The white tin bulk structure is shown in Fig. 1. It may be considered as a body-centered tetragonal lattice with two atoms per unit cell [2].

A group theoretical analysis for the symmetry of the white tin had been presented earlier [3–5].

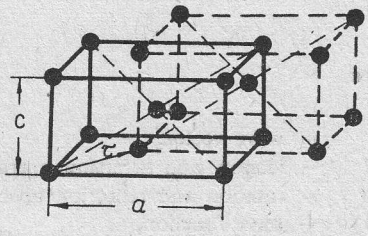

Fig. 1. Crystal lattice of white tin

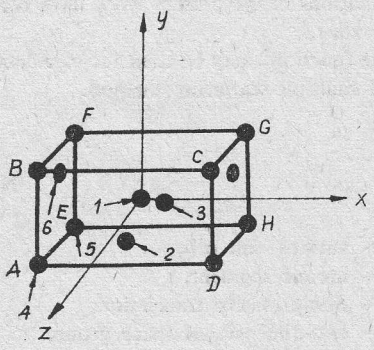

Fig. 2. The surface unit cell

The space group of lattice, besides the primitive translation, contains a set of 16 covering operations, which are pure rotations and reflections, as well as rotations and reflections followed by a non-primitive translations.

Now consider a film of white tin lattice with three atomic layers parallel to the $x-y$ plane. The film which is periodic in two dimensions may be divided into surface unit cells (SUC) as shown in Fig. 2. Such division is used in the multiple-scattering technique [6–8].

The coordinate system is oriented so that z is normal to the surface, whereas x and y are parallel to it. The SUC in two dimensions is spanned by two shortest lattice vectors $\vec{a}=a\vec{i}$ and $\vec{c}=c\vec{j}$ which are parallel to the surface. The quantities a and c denote the structure constants of crystal lattice, and $\vec{i}$, $\vec{j}$ denote the unit vectors.

Along the z axis the SUC is extending over certain number of empty layers. The SUC and its translated counterparts fill the entire space.

The part of SUC to which atoms are confined is called the atomic segment (AS) which we denoted by letters *ABCDEFGH* as shown in Fig. 2. The AS of the SUC contains two atoms from every atomic layer. Each of the six atoms which belong to the AS are denoted by arrows as shown in Fig. 2.

The presence of two atoms per atomic layer introduces some symmetry operations involving the non-primitive translation $\vec{\tau}=1/2\,(\vec{ai})+1/4\,(\vec{cj})$ connecting the two atoms.

Since the film has translational symmetry in two dimensions in the plane of the surface instead of three dimensions, the symmetry of the two-dimensional space group G^s is re-

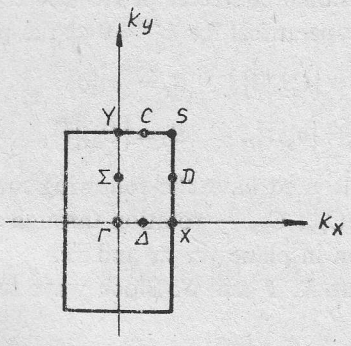

Fig. 3. The two-dimensional BZ

duced when compared with the symmetry of space group G of the bulk crystal. It can be seen in Fig. 2 that the two-dimensional space group besides translational symmetry contains four symmetry elements which leave the lattice invariant.

They are:

$$A_1=\{E|0\} \quad \text{the identity operation},$$
$$A_2=\{\sigma_x|0\} \quad \text{reflection in plane } yz, \tag{2.1}$$
$$A_3=\{\sigma_y|\vec{\tau}\} \quad \text{and} \quad A_4=\{C_{2z}|\vec{\tau}\} \quad \text{reflection}$$

in plane zx and rotation through π about $0z$ followed by a non-primitive translation vector $\vec{\tau}$.

The two-dimensional Brillouin zone (BZ) and the irreducible segment for $x-y$ surface of white tin are shown in Fig. 3 [9]. The vectors specifying the direct and the reciprocal lattices are

$$\vec{R}_m=m_1\vec{a}+m_2\vec{c}, \tag{2.2}$$

$$\vec{G}_n=n_1\vec{b}_1+n_2\vec{b}_2, \tag{2.3}$$

where m_1, m_2, n_1, n_2 are integers and $\vec{b}_1$, $\vec{b}_2$ are reciprocal lattice vectors.

For any distinct wave vector $\vec{k}^s$, there is a group of symmetry operations which are denoted by $P(\vec{k}^s)$. For a given two-dimensional space group G^s the group $P(\vec{k}^s)$ consists of all these point group operations R_i for which

$$R_i\vec{k}^s=\vec{k}^s+\vec{G}_n, \tag{2.4}$$

where $R_i|\vec{\tau}$ is contained in G^s.

For the wave vectors labelled by Γ, X, Y and S there are the following symmetry elements of the group $P(\vec{k}^s)$ [9]:

$$\{E\},\{\sigma_x\},\{\sigma_y\},\{C_{2z}\}. \tag{2.5}$$

The coordinates of the symmetry points are $\Gamma(0, 0)$, $X(\pi/a, 0)$, $Y(0, \pi/c)$ and $S(\pi/a, \pi/c)$.

The film has inversion symmetry but inversion is not a member of the group of the two-dimensional wave vector $\vec{k}^s$ except at the point Γ of the two-dimensional BZ.

In view of the three-dimensional character of AS and the inversion symmetry of the film there are eight symmetry operations for $k^{\rightarrow s}=0$ at the point Γ.

$$\begin{aligned} &B_1=\{E|0\}, \quad B_2=\{C_{2y}|0\}, \quad B_3=\{\sigma_x|0\}, \quad B_4=\{\sigma_z|0\}, \\ &B_5=\{I|\vec{\tau}\}, \quad B_6=\{\sigma_y|\vec{\tau}\}, \quad B_7=\{C_{2z}|\vec{\tau}\}, \quad B_8=\{C_{2x}|\vec{\tau}\}, \end{aligned} \tag{2.6}$$

where the point group symbols used have the following meaning: E, I-the identity and the inversion operations; C_{2y}, C_{2z}, C_{2x} – rotation through π about $0y$, $0z$ and $0x$ respectively; σ_x, σ_z, σ_y – reflection in plane yz, yx and zx.

Now we consider the points X, Y and S. Bloch wave functions at these points may be written [4, 10]

$$\psi_x=\exp(ix\pi/a)u_x(\vec{r}), \quad \psi_y=\exp(iy\pi/c)u_y(\vec{r}) \tag{2.7}$$

and

$$\psi_s=\exp\left[i\left((\pi/a)x+(\pi/c)\,y\right)\right]u_s(\vec{r}), \tag{2.8}$$

where $u_x(\vec{r})$, $u_y(\vec{r})$ and $u_s(\vec{r})$ are periodic functions with period a and c.

All transformations of the form $\vec{t}_1=(2m_1a\vec{i}, m_2c\vec{j})$ are represented by the unit matrix $\{E|\vec{t}_1\}$ since $\exp(i\vec{k}_x^s\cdot\vec{t}_1)=1$ and the transformations $\vec{t}_2=[(2m_1+1)\,a\vec{i}, m_2c\vec{j}]$ are represented by $\{E|\vec{t}_2\}$ where $\exp(i\vec{k}_x^s\cdot\vec{t}_2)=-1$.

At the point X the operator A_3^2 must be included in the group of this wave vector. A_3^2 commutes with every element of the group given by (2.1). Thus the group of this wave vector is of order 8 and has the following symmetry elements:

$$\begin{aligned} &C_1=\{E|\vec{t}_1\}, \quad C_2=\{\sigma_x|\vec{t}_1\}, \quad C_3=\{\sigma_y|\vec{\tau}+\vec{t}_1\}, \quad C_4=\{C_{2z}|\vec{\tau}+\vec{t}_1\}, \\ &C_5=\{E|\vec{t}_2\}, \quad C_6=\{\sigma_x|\vec{t}_2\}, \quad C_7=\{\sigma_y|\vec{\tau}+\vec{t}_2\}, \quad C_8=\{C_{2z}|\vec{\tau}+\vec{t}_2\}. \end{aligned} \tag{2.9}$$

By means of similar analysis we obtain the elements of the groups D and F of the wave vectors Y and S respectively

$$\begin{aligned} &D_1=\{E|\vec{t}_3\}, \quad D_2=\{\sigma_x|\vec{t}_3\}, \quad D_3=\{\sigma_y|\vec{\tau}+\vec{t}_3\}, \quad D_4=\{C_{2z}|\vec{\tau}+\vec{t}_3\}, \\ &D_5=\{E|\vec{t}_4\}, \quad D_6=\{\sigma_x|\vec{t}_4\}, \quad D_7=\{\sigma_y|\vec{\tau}+\vec{t}_4\}, \quad D_8=\{C_{2z}|\vec{\tau}+\vec{t}_4\}, \end{aligned} \tag{2.10}$$

where $\vec{t}_3=(m_1a\vec{i}, 4m_2c\vec{j})$ and $\vec{t}_4=[m_1a\vec{i}, (4m_2+1)\,c\vec{j}]$.

$$\begin{aligned} &F_1'=\{E|\vec{t}_5'\}, \quad F_2'=\{\sigma_x|\vec{t}_5'\}, \quad F_3'=\{\sigma_y|\vec{\tau}+\vec{t}_5'\}, \quad F_4'=\{C_{2z}|\vec{\tau}+\vec{t}_5'\}, \\ &F_5'=\{E|\vec{t}_6'\}, \quad F_6'=\{\sigma_x|\vec{t}_6'\}, \quad F_7'=\{\sigma_y|\vec{\tau}+\vec{t}_6'\}, \quad F_8'=\{C_{2z}|\vec{\tau}+\vec{t}_6'\} \end{aligned} \tag{2.11}$$

or an eqivalent set symmetry elements

$$\begin{aligned} &F_1''=\{E|\vec{t}_5''\}, \quad F_2''=\{\sigma_x|\vec{t}_5''\}, \quad F_3''=\{\sigma_y|\vec{\tau}+\vec{t}_5''\} \quad F_4''=\{C_{2z}|\vec{\tau}+\vec{t}_5''\}, \\ &F_5''=\{E|\vec{t}_6''\}, \quad F_6''=\{\sigma_x|\vec{t}_6''\}, \quad F_7''=\{\sigma_y|\vec{\tau}+\vec{t}_6''\}, \quad F_8''=\{C_{2z}|\vec{\tau}+\vec{t}_6''\} \end{aligned} \tag{2.12}$$

where $\vec{t}_5'=(2m_1\,a\vec{i}, 4m_2\,c\vec{j})$, $\vec{t}_6'=[(2m_1+1)\,a\vec{i}, 4m_2\,c\vec{j}]$ and

$$\vec{t}_5''=[(2m_1+1)\,a\vec{i}, 4(m_2+1)\,c\vec{j}], \vec{t}_6''=[2m_1\,a\vec{i}, (4m_2+1)\,c\vec{j}].$$

The groups of the wave vectors Γ and Y are of order 8. Each operation forms a class by itself and the classes are non-degenerate.

The groups of the wave vector X and S are also of order 8 and contain five classes. There are four non-degenerate and one doubly-degenerate states.

For example, the classes of the group of the wave vector X are as follows:

$$\varepsilon_1=C_1, \quad \varepsilon_2=C_5, \quad \varepsilon_3=C_2+C_6, \quad \varepsilon_4=C_3+C_7, \quad \varepsilon_5=C_4+C_8. \tag{2.13}$$

3. The calculation of the character tables

The first step in the calculation of the character table is the determination of the class multiplication coefficients C_{ijs}. The product of two classes can be expanded as linear combinations of classes in the following way:

$$\varepsilon_i\varepsilon_j=\sum_s C_{ijs}\varepsilon_s. \tag{3.1}$$

The replacement of classes by their characters leads to the formula

$$h_i h_j \chi_i \chi_j=\chi_E \sum_s C_{ijs} h_s \chi_s, \tag{3.2}$$

where h_i, h_j, h_s denote the number of elements of symmetry in classes i, j, s respectively, and χ_i, χ_j, χ_s denote the corresponding characters, wheraes χ_E is the character of the matrix defining the identity operation.

A quantity X_j is introduced by the equation

$$X_i\chi_E=h_i\chi_i. \tag{3.3}$$

Equation (3.2) expressed in terms of X_i took the form given in [10]

$$\sum_{s=1}^{r}(C_{ijs}-X_j\delta_{is})X_s=0. \tag{3.4}$$

For fixed j the condition for the existence of finite solution is

$$\begin{vmatrix} C_{1j1}-X_j & C_{1j2} & \dots & C_{1jr} \\ C_{2j1} & C_{2j2}-X_j & \dots & C_{2jr} \\ \dots & \dots & \dots & \dots \\ C_{rj1} & \dots & \dots & C_{rjr}-X_j \end{vmatrix}=0. \tag{3.5}$$

The number of classes is denoted by r, and therefore for each class there are r roots. The r determinantal equations solution of which for each j provides values of X_j. From these values of X_j it is necessary to derive the corresponding characters χ_i from the equation (3.3). The orthogonality relations are needed to get the proper sequence of charac-

Table 1

Character system for the point Γ

Γ	$\{E\|0\}$	$\{C_{2y}\|0\}$	$\{\sigma_x\|0\}$	$\{\sigma_z\|0\}$	$\{I\|\vec{\tau}\}$	$\{\sigma_y\|\vec{\tau}\}$	$\{C_{2x}\|\vec{\tau}\}$	$\{C_{2z}\|\vec{\tau}\}$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	−1	−1	1	1	−1	−1
Γ_3	1	−1	−1	1	1	−1	−1	1
Γ_4	1	−1	1	−1	1	−1	1	−1
Γ_5	1	1	1	1	−1	−1	−1	−1
Γ_6	1	1	−1	−1	−1	−1	1	1
Γ_7	1	−1	−1	1	−1	1	1	−1
Γ_8	1	−1	1	−1	−1	1	−1	1

ters down a given vertical column. The order in which the rows occur in the character table is arbitrary or conventional.

For all irreducible representations of a group one must take into account the orthogonality relations [12].

In tables 1 and 2 are given the character tables for the two-dimensional space group of white tin and for wave vectors referring to the Γ and X points in the two-dimensional BZ.

For the representations X_5 and S_5 which are two-dimensional, instead of characters, all the irreducible matrices have been evaluated. Since all the matrices of the point group

Table 2

Character system associated with the point X

X	$\{E\|\vec{t}_1\}$	$\{\sigma_x\|\vec{t}_1\}$	$\{\sigma_y\|\vec{\tau}+\vec{t}_1\}$	$\{C_{2z}\|\vec{\tau}+\vec{t}_1\}$	$\{E\|\vec{t}_2\}$	$\{\sigma_x\|\vec{t}_2\}$	$\{\sigma_y\|\vec{\tau}+\vec{t}_2\}$	$\{C_{2z}\|\vec{\tau}+\vec{t}_2\}$
X_1	1	1	1	1	1	1	1	1
X_2	1	−1	1	−1	1	−1	1	−1
X_3	1	1	−1	−1	1	1	−1	−1
X_4	1	−1	−1	1	1	−1	−1	1
X_5	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\-1&0\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}0&1\\-1&0\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$

commute with each other, a single transformation matrix S can be found such that each matrix undergoing a similarity transformation by S becomes diagonal. Thus we have considered tables for irreducible representations for a given wave vector $\vec{k}^s$.

These representations can be used to provide a scheme for labelling the electronic states, as well as to identify any essential degeneraces and to simplify the calculation of band structures. The analysis for other wave vectors can follow the same line.

4. The generation of symmetry-adapted functions

Having determined the character tables, we are now able to find all possible symmetry-adapted functions that belong to each of the representations. These functions have correct properties required by the representation under transformation by the group elements. The operators which accomplish this process are known as projection operators and are defined as [11, 13–15]

$$P^{p}_{mn}=\exp(i\vec{k}^{s}\cdot\vec{t}_{1,2})\,l_p/g\sum_{R}\Gamma^{\alpha}(R)^{*}_{mn}P(R) \tag{4.1}$$

and

$$P^{p}=\exp(i\vec{k}^{s}\cdot\vec{t}_{1,2})\,l_p/g\sum_{R}\chi^{\alpha}(R)^{*}P(R). \tag{4.2}$$

We form such operations which belong to each irreducible representation. For the generating functions we take spherical harmonics for $l_{\max}=4$. In order to proceed further we need also expressions for $RY_{lm}(\vec{r})$.

The projection operators (4.1) and (4.2) applied to the one-dimensional representations at Γ and Y and to two-dimensional representation at X and S give the linear combinations of basis functions for a particular representation. The results are shown in table 3.

Table 3

Symmetry-adapted functions at Γ and Y

l	Γ	Y	Basis functions
0	Γ_1	Y_1	Y_{00}
1	Γ_5	Y_5	Y_{10}
1	Γ_7	Y_7	$1/\sqrt{2}(Y_{1-1}+Y_{11})$
2	Γ_1	Y_1	$1/\sqrt{3}(Y_{20}+Y_{2-2}+Y_{22})$
2	Γ_3	Y_3	$1/\sqrt{2}(Y_{2-1}+Y_{21})$
3	Γ_5	Y_5	$1/\sqrt{3}(Y_{30}+Y_{3-2}+Y_{32})$
3	Γ_7	Y_7	$1/\sqrt{4}(Y_{3-1}+Y_{31}+Y_{3-3}+Y_{33})$
4	Γ_1	Y_1	$1/\sqrt{5}(Y_{40}+Y_{4-2}+Y_{42}+Y_{4-4}+Y_{44})$
4	Γ_3	Y_3	$1/\sqrt{4}(Y_{4-1}+Y_{41}+Y_{4-3}+Y_{43})$

The representations X_5 and S_5 have dimension greater than 1, which arises when the symmetry group contains non-commuting elements leading to the possibility of degeneracy. In this case we obtain two independent sets of symmetry-adapted functions which form bases of this representation. These functions are given in table 4.

Table 4

Symmetry-adapted functions at X and S

l	X	S	Basis functions
0	X_5^1	S_5^1	Y_{00}
1	X_5^1	S_5^1	Y_{10}
1	X_5^2	S_5^2	$1/\sqrt{2}(Y_{1-1}+Y_{11})$
2	X_5^1	S_5^1	$1/\sqrt{3}(Y_{20}+Y_{2-2}+Y_{22})$
2	X_5^2	S_5^2	$1/\sqrt{2}(Y_{2-1}+Y_{21})$
3	X_5^1	S_5^1	$1/\sqrt{3}(Y_{30}+Y_{3-2}+Y_{32})$
3	X_5^2	S_5^2	$1/\sqrt{4}(Y_{3-1}+Y_{31}+Y_{3-3}+Y_{33})$
4	X_5^1	S_5^1	$1/\sqrt{5}(Y_{40}+Y_{4-2}+Y_{42}+Y_{4-4}+Y_{44})$
4	X_5^2	S_5^2	$1/\sqrt{4}(Y_{4-1}+Y_{41}+Y_{4-3}+Y_{43})$

We see that nothing goes with Γ_2, Γ_4, Γ_6, Γ_8 and Y_2, Y_4, Y_6, Y_8 as well as X_1, X_2, X_3, X_4 and similarly with S_1, S_2, S_3 and S_4.

We have evaluated the functions $\mathscr{Y}_{lm}(\vec{r})$ which are linear combinations of spherical harmonics of angular momentum l, with argument the angular coordinates of $\vec{r}$. These combinations are chosen such that they transform under the irreducible representations of the symmetry group of wave vector $\vec{k}^s$. They are normalized, real and mutually orthogonal.

Instead of expanding the wave functions around each center j, within the AS, in ordinary spherical harmonic we can expand them in linear combinations of functions $\mathscr{Y}_{lm}(\vec{r})$.

$$\psi(\vec{r}) = \sum_{l=0}^{l} C_{lm}^{(j)} R_l(r_j) \mathscr{Y}_{lm}(\vec{r}_j), \quad j=1, \ldots, 6 \tag{4.3}$$

which are basis for the various irreducible representations. This can be used to simplify the form of $\psi(\vec{r})$ and reduce the number of structure constants which appear in calculations of the band structures by means of multiple-scattering method.

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References

[1] J. A. Appelbaum, D. R. Hamann, *The electronic structure of solid surfaces.* Rev. Mod. Phys., Vol. 48, p. 479, 1976.

[2] J. E. Craven, *Band structure and Fermi surface of white tin as derived from de Haas-van Alphen data.* Phys. Rev. Vol.182, p. 693, 1969.

[3] S. Mase, *Algebraic method to obtain irreducible representations of space groups with an application to white tin.* J. Phys. Soc. Japan, Vol. 14, p. 1538, 1959.

[4] M. Miąsek, M. Suffczyński, *Space group of white tin. 1. Symmetry points.* Bull. Acad. Polon. Sci. Ser. Sci. Math. Astron. Phys., Vol. 9, p. 477, 1961.

[5] M. Suffczyński, *Space group of white tin. 3. Double group.* Bull. Acad. Polon. Sci. Ser. Sci. Math. Astron. Phys., Vol. 9, p. 489, 1961.

[6] W. Kohn, *Green's-function method for crystal films and surfaces.* Phys. Rev., Vol., B11, p. 3756, 1975.

[7] N. Kar, P. Soven, *Band structure of thin films.* Phys. Rev., Vol. B11, p. 3761, 1975.
[8] W. Drabowicz, *Multiple-scattering method for crystal surface.* Acta Phys. Pol., Vol. A56, p. 355, 1979.
[9] A. P. Cracknell, *Tables of the irreducible representations of the 17 two-dimensional space groups and their relevance to quantum mechanical eigenstates for surfaces and thin films.* Thin solid films, Vol. 21, p. 107, 1974.
[10] H. Jones, *The theory of Brillouin zones and electronic states in crystals.* 2nd. ed., North-Holland, Amsterdam 1975.
[11] V. Heine, *Group theory in quantum mechanics.* Pergamon Press, London, Oxford, New York, Paris 1960.
[12] M. Tinkham, *Group theory and quantum mechanics.* McGraw-Hill, New York, San Francisco, Toronto, London 1964.
[13] S. L. Altmann, A. P. Cracknell, *Lattice harmonics 1. Cubic groups.* Rev. Mod. Phys., Vol. 37, p. 19, 1965.
[14] J. F. Cornwell, *Group theory and electronic energy bands in solids.* North-Holland, Amsterdam, London 1969.
[15] C. J. Bradley, A. P. Cracknell, *The mathematical theory of symmetry in solids.* Clarendon Press, London 1972.

Symetryczne funkcje falowe dla powierzchni kryształu

Streszczenie

W niniejszej pracy przeprowadzono analizę grupowo-teoretyczną powierzchni (100) kryształu białej cyny.

Na podstawie odpowiednich obliczeń wyznaczono tabele charakterów oraz funkcje falowe transformujące się zgodnie z reprezentacjami nieredukowalnymi dla grupy wektorów odpowiadającej czterem punktom Γ, X, Y i S dwuwymiarowej strefy Brillouina.

Funkcje te stosowane są do analizy ilościowej struktury pasmowej powierzchni kryształu traktowanego w ramach modelu cienkiego filmu.

Базисные волновые функции для поверхности кристалла

Резюме

Таблицы характеров, а также базисные волновые функции, были расчитаны для двумерной несимморфной пространственной группы соответствующей поверхности (100) белого олова.

Расчеты были ограничены для четырех волновых векторов Γ, X, $У$ и S поверхностной зоны Бриллюэна.

Базисные функции могут быть использованы для расчетов электронных свойств тонких и толтых кристаллических фильмов методом многократного рассеяния.