ELECTRON ENERGY BANDS IN SEMICONDUCTOR FILMS

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The possible nature of the band structure in crystal films is examined on the basis of a consideration of the symmetry possessed by their structure.

For germanium and silicon of the p- and n-types with various different orientations of the film the connection is found between the band structures of the film and of the bulk crystal. The result is obtained that with the orientation [111] an n-germanium film, like an n-silicon film with the same orientation must have a single-trough minimum.

The overlapping can be absent only in the case of very thin films with pronounced anisotropy.

Translational symmetry in a crystal leads, as we know, to band characteristics in the energy spectrum of the quasi-particles, in particular, of the current carriers—electrons and holes. In each band the energy is a continuous function of the quasi-momentum \( \kappa \) whose values lie in the Brillouin zone, namely 

\[ \varepsilon(\kappa_x, \kappa_y, \kappa_z). \]

The theory of representations of Fedorov symmetry groups of crystals enables us to clarify the characteristic peculiarities of the band structure [1], and additional use of the theory of perturbations enables us to find the form of \( \varepsilon(\kappa) \) near the edge of the energy band [2].

The results of research into the band structure of semiconductor crystals can be found in the reviews [3, 4].

PECULIARITIES OF BAND STRUCTURE CAUSED BY THE BOUNDEDNESS OF THE FILM

In the transition from the bulk crystal to the crystal film the nature of the band structure is certain to change to some extent. Because of the boundedness of the film in one dimension the transverse projection of the quasi-momentum is not a better quantum number and has an indeterminacy of \( \sim 2\pi/L \), where \( L \) is the thickness of the film. So the states and energies of the electrons and holes (quasi-particles in general) are given by the longitudinal projections \( \kappa_x \) and \( \kappa_y \) and the discrete quantum numbers \( n \) which replace \( \kappa_z \). As a result quasi-discrete levels \( \varepsilon(\kappa_x, \kappa_y, n) \)—sub-bands—appear. The energy difference between neighboring sub-bands for fixed \( \kappa_x \) and \( \kappa_y \) is equal in order of magnitude to the change in the energy of an electron in a bulk crystal when \( \kappa_z \) varies by a quantity of indeterminacy \( \sim 2\pi/L \). Such an estimate can have meaning while the film contains many atomic layers. The width of the sub-bands due to the dependence of \( \varepsilon \) on \( \kappa_x \) and \( \kappa_y \) is as a rule greater than the difference between the sub-bands since the region of variation of \( \kappa_x \) and \( \kappa_y \), equal to \( 2\pi/a \) \((a\) being the lattice constant), is much greater than the indeterminacy of \( \kappa_z \), so the sub-bands must overlap considerably.

The overlapping can be absent only in the case of very thin films with pronounced anisotropy.

The dependence of the electron energy in the film on the discrete number \( n \) leads to many physical effects [5, 8]. In particular this discreteness is important when the electrons are located mainly in states of only one lower sub-band (holes in the upper sub-band). In this case the space of electron states can be regarded as two-dimensional although the crystal film itself is a particularly three-dimensional formation \((L \gg a)\). This case is often realized in practice in the semiconductor films which are obtained [5].

The nature of the sub-bands in crystal films can in principle be studied by the methods of group theory as in the case of a bulk crystal. However it should be borne in mind that the symmetry of the film's structure contains only translations lying in the plane of the film. In what follows we shall, in contrast to the case of a bulk crystal, call a system of translations in a crystal film not a lattice but a grid of translations. Of the rotational symmetry elements only those are possible which transfer onto itself the translation grid which is obtained. Thus in the transition from the bulk crystal to the crystal film the symmetry group passes over from the Fedorov group to one of the 80 two-dimensional symmetry groups (a list and description of of them may be found in [6]). In our case the motif which is transmitted by the plane grid is the group of atoms which extends over the whole thickness of the film.

The energy levels in the film are given by irreducible representations of the two-dimensional space group which are determined in the same way as the representations of the Fedorov groups—by giving the star of the two-dimensional quasi-momentum and by small representation.

The change in the energy connected with the passage of the star of the wave vector through all possible values of the plane Brillouin zone gives one sub-band. It should be noted that, while the two-dimensional translational symmetry of the film is a subgroup of the translational symmetry of the crystal, the reciprocal lattice (grid) of the film does not possess an analogous property. To a certain extent the opposite situation is the case—the vectors of the reciprocal lattice of the crystal which are parallel to the plane of the film form a subgroup of the group of the two-dimensional reciprocal grid. This leads to the situation where the two-dimensional Brillouin zone for the crystal film is inside the plane which is formed by the translations of the reciprocal lattice of the crystal which are parallel to the plane of the film. This circumstance is important in considering the connection between the band structure of the crystal film and that of the bulk crystal.

As we have already noted, the crystal film is a three-dimensional formation, and it contains many
atomic layers. Therefore the nature of the sub-bands must be connected with the band structure of the bulk crystal. This connection can be taken into account by considering the boundedness of the film in one direction as a small perturbation. In order to obtain the energy levels which must exist in the film it is necessary to decompose the irreducible representation of the Fedorov group into irreducible representations of the symmetry group of the film's structure.

We shall first make some remarks. In translational transformations which belong to the symmetry group H of the film's structure, the basis functions of the initial irreducible representation \( \Gamma_k \) of the symmetry group of the bulk crystal are multiplied by the quantity \( \exp[i(x \kappa_x + y \kappa_y)] \). This means that there will be in the decomposition of \( \Gamma_k \) only those irreducible representations of \( H \) whose basis functions can be obtained by projecting the star of \( \Gamma_k \) into the plane of the film. Here the projections of the irreducible star of \( K \) can form one or several irreducible stars relative to the two dimensional space group.

It may turn out that not all projections of \( K \) with the same \( \kappa_x \) lie in the first plane Brillouin zone. This means that the continuous energy function depending on \( \kappa_x \) and \( \kappa_y \) suffers a discontinuity on transition from the bulk crystal in the crystal film at points on the boundary of the first Brillouin zone, and this leads to the appearance of a new sub-band. The result is obtained that the boundedness of the dimensions of the film in the z direction can in principle lead to a qualitative change in the motion of an electron along the film—a discontinuity in \( \varepsilon(\kappa_x, \kappa_y) \).

In order to avoid misunderstanding we remark that everywhere in the present article what we are discussing is electron or hole states in which the electron density is distributed throughout the whole volume of the film. The surface states which are in principle bulk crystal in the crystal film at points on the boundary are not considered in the present article.

We now go on to consider concrete examples of semiconductor crystals. Our interest will be centered on the edge of the conduction band—lower sub-band, and the edge of the valence band—upper sub-band. 

**Symmetry of Germanium and Silicon Films: Two Dimensional Brillouin Zones**

Although the conduction bands of germanium and silicon differ markedly, we shall consider Ge and Si together, bearing in mind the fact that they have identical symmetry. The most frequently encountered direction of growth of Ge and Si films is [111]; two other directions of growth, characteristic of cubic crystals are also possible—[001] and [011].

The symmetry of Ge and Si forms the group \( O_h^1 \), in which the Bravais lattice is a face-centered cube, \( F_c^0 \).

When the normal to the film is oriented along [001] there remains of the fundamental translations \( F_c^0 \) only \( a_0 = d(1/2 0 1/2) \), directed along the base diagonal of the cube (here \( d \) is the length of a side of the cube). We shall take this translation as a fundamental translation in the two-dimensional lattice \( a_2 = a_0 \). The other fundamental translation will be directed along the second base diagonal \(-a_2 = a_1 - a_2 = d(-1/2 1/2 0)\). As a result we obtain for the translational symmetry of the film a square non-centered grid (in the two-dimensional case the square grid is always noncentered). The reciprocal grid is also square, with the basis vectors

\[
\beta_1 = \frac{2\pi}{d} (-1, 1, 0), \quad \beta_2 = \frac{2\pi}{d} (0, 1, 1).
\]

Of the rotational symmetry elements (including the symmetry with respect to reflections) there remain the vertical planes which pass through the fundamental translations and the horizontal axes of the second order along the x and y axes. There are no screw axes or glide planes in the symmetry group. As a result we obtain the group \( D_{2d} \). The complete symmetry of the structure of the film is a two-dimensional space group which in [6] has the number 78.

When the normal to the film is oriented along [110], it is necessary to take as the fundamental translation the translation along the plane diagonal of the cube \( a_1 = a_2 = d(-1/2 1/2 0) \) and the vertical translation \( a_2 = a_1 + a_2 = a_3 = d(001) \). The translational symmetry represents an orthorhombic noncentered grid. It is easy to obtain the basis vectors of the reciprocal grid

\[
\beta_1 = \frac{2\pi}{d} (001), \quad \beta_2 = \frac{2\pi}{d} (-110).
\]

The Brillouin zone represents a rectangle the smaller side of which \((2\pi/d) \cdot (1/2)\) is directed along [001] and the large side \((2\pi/d) \cdot (\sqrt{2}/2)\) along the base diagonal of the cube.

Of the rotational elements of the group \( O_h^1 \) those with the given orientation remaining on the transition to the film are the axis of the second order along [001] and the two \( \sigma_{xy} \). They constitute the group \( C_{4v} \). The complete symmetry group has the number 13 in [6].

We pass on to the task of determining the symmetry of the structure of a crystal film perpendicular to the space diagonal of the cube. We take the normal to the film along [−111]. With this choice the fundamental translations of the three-dimensional lattice \( a_2 = d(1/2 0 1/2) \) and \( a_3 = d(1/2 1/2 0) \) lie in the plane of the film and can be taken as the fundamental translations \( a_1 \) and \( a_2 \) of the plane grid. The translations \( a_1 \) and \( a_2 \) are equal in magnitude and make an angle of 60° with one another. Thus the grid is hexagonal. The basis vectors of the reciprocal grid, determined in the usual way, are

\[
\beta_1 = \frac{2\pi}{d} \left( \frac{2}{3}, 1, 1 \right), \quad \beta_2 = \frac{2\pi}{d} \left( \frac{2}{3}, 1, -1 \right).
\]

The symmetry of the structure of the film is determined as in the preceding cases. The rotational symmetry forms the group \( D_{3d} \), and the complete symmetry forms group no.78.