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Kinetic Description of Propagation of Quasiparticles Fluxes in Solid-state Structure

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Abstract: Within the framework of the kinetic theory, the interaction of systems of quasiparticles and the exchange of quasiparticles of different types between layers of a plane-parallel solid structure are taken into account. The reasons influencing the propagation of differential fluxes of quasiparticles near each boundary of the structure are indicated. These include not only the appearance of a force field, in particular, electric $e\nabla\varphi(x)$ and thermal $\nabla T(x)$, fields near the boundary in equilibrium and its modification when equilibrium is disturbed, but also a change in the coordinate and angular dependence of the relaxation length of fluxes $l_e(x, k, \Omega)$ in the same region. Some modification of the distribution of characteristic thermodynamic quantities in the inhomogeneous region of the layer in comparison with the homogeneous layer also affects the propagation of fluxes. The necessity of a self-consistent solution of the kinetic boundary value problem of the joint propagation of differential fluxes of quasiparticles-a system of equations and integral boundary conditions-is substantiated. Near the boundary and in another inhomogeneous region of the layer thickness, as well as in the thin layer as a whole, in quasiparticles systems, it is proposed to use a specific coordinate distribution of the flux density of thermodynamic quantities over the structure thickness, which is mutually self-consistent with the propagation of the corresponding quasiparticles fluxes. The main conclusion of this work: when developing modern multilayer solid-state structures, especially with thin layers, it is necessary to use the kinetic theory, which adequately takes into account the physical picture that occurs not only in homogeneous and inhomogeneous regions of the thickness of each layer, but also at all boundaries of the structure.

***Keywords*:** solid-state layers, boundaries, quasiparticles, fluxes distribution, thermodynamic values

1. Introduction

Modern solid-state structures, in particular solar cells [1], photodetectors [2], light-emitting diodes [3], lasers [4] and many other electronic devices [5], usually consist of several solid-state layers of different atomic composition or phase structures and doping. Such layers have different physical properties. An optimized structure for any purpose is characterized by a set of material properties of its layers, their location in the structure and thickness. Each layer has its own specific thickness, mutually consistent with other layers, in its structure, possibly micron, submicron, nano-scale, or even atomic.

Structures are usually created in a monolithic "multi-layer" and are generally heterogeneous environments. Thus,

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modern structures can contain different solid-state materials with their own specific electrical, optical, thermal, etc. properties. The boundaries between layers (solid materials) also have their own specific properties. These boundaries can have a significant effect on the properties of the solid layers that make up the structure and on the physical characteristics of the structure as a whole, especially if the structure contains thin layers. The efficiency of functioning and the cost of the structure and the electronic device as a whole depend on the successful choice of the initial solid-state materials, the technological perfection of the layers grown in the structure and the boundaries between them (and contacts), as well as on the correct choice of the optimal dimensions of the layer thickness.

Any solid layer is a complex quantum mechanical object that contains a huge variety of particles of different types. An even more complex multiparticle object is an inhomogeneous (multilayer) monolithic structure. When studying certain properties of a layer or structure (for example, electrical ones), one "main" system is usually distinguished, (in particular, an electron-hole one), which is also many-particle. To simplify, from a many-particle theoretical description, one passes to a one-particle physical and mathematical theory (for example, [6]) with a qualitative account of statistics. Along with the electron-hole system, it is similarly justified to distinguish some other systems of quasiparticles of solid materials [7-10]: phonon, photon, and others, whose role in the phenomenon under study is important. They also use their own one-particle theoretical description and statistics.

The functioning of many electronic devices, including solar cells, light-emitting diodes, lasers, thermos-elements and others, is based on the interaction of systems of charge carriers, photons, phonons, and quasiparticles of other types, which occurs in the layers of a solid-state structure. Thus, in a solar cell, photons that have entered (possibly scattered) into the layers of the structure become excess internal radiation, which excites the electron and/or hole systems in the layers, as well as (directly and indirectly) systems of phonons of acoustic and optical branches and, possibly, other systems. In the layers, there is a decrease in these fluxes of photons and the energy transferred by them, which leads to the appearance of excess (no equilibrium) fluxes of charge carriers and fluxes of quasiparticles of other types. In this case, as a result of a decrease in a specially "technologically" created internal electric potential, which is located in one or some layer(s) of the structure (or at the boundary), an "external" electric potential appears at the contacts of the cell structure. If the contacts are connected, for example, through a payload, then a current appears in the circuit. The magnitude of this current depends on many factors, including the mode of operation of the solar cell ("short circuit", under some load or "no-load" [5, 7])

In reality, technological methods create a certain inhomogeneous region in the structure, for example, a *p*-*n*-junction in a layer, or a heterojunction, or simply a contact of solid-state layers, or a combination of them. And the propagation of internal elementary multidirectional (differential) equilibrium fluxes of charge carriers [11], phonons, photons and quasiparticles of other types [12] is created due to changes in the conditions of their propagation in and near an inhomogeneous region, for example, near a contact (boundary) or *p*-*n*-junction, internal force fields. These fields, in particular electric [10] and thermal [12], act not only on equilibrium, but also on no equilibrium (in particular, excess) quasiparticles. The appearance of excess fluxes of charge carriers and quasiparticles of other types (directed towards and away from the local inhomogeneous region) changes the magnitude of the internal fields. In this case, a certain potential difference arises at the contacts of the structure.

In the layers of the LED structure, excited by an external electric potential difference at its contacts, the system of injected electrons emits photons (as well as phonons and possibly other types of quasiparticles), some of which go out [5]. In this case, the energy from the system of electrons is transferred to streams of photons and of quasiparticles of other types. Obviously, the more excitation is transmitted for the intended purpose of the structure, the more efficiently it functions. Due to the difference in the physical properties of various solid-state materials from which it is possible to make (of different thicknesses) layers of a structure for one purpose or another, the fractions of the useful redistribution of primary excitation in them can differ significantly (as well as the cost of the structure as a whole).

Of course, in order to construct an optimized structure for all layers of which it will consist (in atomic composition or phase structure, in the degree of their alloying, i.e. in the physical properties of solid-state materials in general, as well as in the thickness of each layer and properties boundaries), it is necessary to understand well, or at least adequately, the whole physical picture taking place in the structure, including around it and on its boundaries. It is difficult to achieve sufficiently deep optimization within the framework of the drift-diffusion theory [5, 7], especially if the structure contains thin layers and many boundaries.

Although in this case for a specific structure it is possible to adjust the parameters (diffusion coefficient, mobility, diffusion length, surface recombination rate, the thickness of the “space charge region”, “height of the potential barrier, etc.) to the experimentally obtained characteristics of this structure, it is rather difficult to explain the reasons for choosing this particular set of parameters. This means that the above description is not entirely adequate, it is only approximate, and largely based on previously experimentally determined (within the framework of the same theory) data.

Previously, within the framework of the kinetic theory, it was shown that many of these parameters depend not only on the properties of a particular layer of a solid-state structure, but also on the presence of adjacent layers of the structure, directly on the properties of its boundaries and on the thickness of the structure layer. These factors are not taken into account in the drift-diffusion theory. It was also pointed out that the properties of a layer in a structure, especially a thin one, may differ in many respects from the properties of an individual layer of the same atomic composition, structure and size. This is due to the difference in the structure and state of the layer boundaries in these cases and the absence of exchange of charge carriers and other quasiparticles in the case of studying the properties of an individual layer. As a result, the experimental data on the properties of an individual layer may differ markedly from the properties of the layer in the structure. As shown above, it is often necessary to take into account the interaction of quasiparticles of different types in the layers of the structure, at least within the framework of the kinetic theory.

The interaction of systems of quasiparticles inherent in a solid medium is carried out by the propagation and scattering of fluxes of different kinds of quasiparticles. The interaction of charge carriers and other quasiparticles in the uniform thickness of each layer and at its boundaries usually differs significantly, both within one system and between systems of quasiparticles of different types [13-15]. The exchange of quasiparticles between the layers of the structure, carried out by multidirectional elementary (differential) fluxes of quasiparticles across the boundary in both directions from it, provides the mutual influence of the layers on their physical properties near the boundary and in equilibrium, and when it is violated. Note that the depth of the region of the layer at which the influence of the boundary is still significant in various systems of quasiparticles can differ markedly. It depends on both internal and external physical conditions. Obviously, the properties of the boundary itself, due to its composition, configuration, and state, affect the exchange of quasiparticles between the layers and, in general, the physical picture that occurs near the boundary. This must be taken into account in the R & D of solid structures, especially multilayer and, moreover, containing thin layers.

The previously developed kinetic theory [13-17], which takes into account the joint propagation of differential fluxes of quasiparticles of different types (the most significant under specific conditions) in all layers of the structure, along with the corresponding computer simulation, in principle, allows you to optimize the design of an effective plane-parallel structure, taking into account the properties of the selected specific initial materials and the resulting properties of the boundaries between them. However, for a more realistic description of the physical picture occurring near the boundaries of each solid layer of the structure, it is also necessary to take into account some circumstances of a statistical and spatial (geometric) nature. A deeper description of the joint propagation of differential fluxes of quasiparticles of different types requires a larger number of parameters and characteristics for each layer of the structure and boundaries. Due to the significant difference in the physical nature of quasiparticles of different types, this is obvious.

For simplicity, here we mainly consider a system of charge carriers in isotropic adjacent solid layers of uniform in thickness. A detailed study of the physical picture of the propagation of differential fluxes of charge carriers near the boundary and across it in the framework of the kinetic theory will allow deeper optimization of the design of a plane-parallel solid structure. Earlier, in the kinetic theory of contact phenomena, the configuration and state of the boundary were either not taken into account at all, or taken into account very approximately [5, 7].

In the case of weak interaction of systems, the properties of a plane boundary on a kinetic scale can be largely characterized by the scattering probabilities of differential fluxes of charge carriers $P(\mathbf{k}, \mathbf{k}_*)$, where $\mathbf{k}$ is the wave vector of the differential flux incident on the boundary, and $\mathbf{k}_*$ is a certain wave vector of the flux scattered by the boundary [13]. Obviously, the incident flux is directed “to the boundary”, and the scattered one-“from the boundary”, either in the considered layer or in the adjacent one. Similarly, on the same boundary, the fluxes are scattered in the neighboring (adjacent) layer, which has its own properties. If the interaction of systems of quasiparticles at the boundary is strong, then to describe the scattering processes it is necessary at least to introduce a matrix composed of $P_{ij}(\mathbf{k}_i, \mathbf{k}_j)$ [13], where the wave vectors $\mathbf{k}_i$ and $\mathbf{k}_j$ can belong to quasiparticles of different types.

The division of differential fluxes in all considered systems into fluxes “to the boundary” and “from the boundary”, for example, $q^+(x, k, \Omega)$ and $q^-(x, k, \Omega)$, is of fundamental importance. Since the boundary probabilities $P(\mathbf{k}, \mathbf{k}_*)$ differ from the "volume" scattering probabilities in the homogeneous layer thickness, symmetric in the isotropic medium, this circumstance should on a miscellaneous effect the character of the spatial distribution of differential fluxes directed "towards the boundary" and "away from the boundary", at least near the border [3], as well as on the interrelated consequences of this.

Within the framework of the kinetic theory, the exchange of charge carriers and quasiparticles of other types, which have different energies ε_i associated with the wave vector $\mathbf{k}_i$, is carried out by their differential fluxes incident on the boundary at different angles. The integral (total) fractions of flows reflected from the boundary, "lost" at the boundary, and passed through the boundary depend not only on the kinetic properties of the layer thickness (where fluxes are mainly formed), but also on the nana-scale configuration and state of the boundary. Obviously, the configuration and state of the boundary are determined both by the atomic properties of the materials of neighboring layers and the mutual orientation of the crystal axes, and in many respects by the technology of growing the structure, including the possible intermediate processing of the boundary.

In an inhomogeneous medium of a structure, multidirectional differential fluxes of charge carriers (and quasiparticles of other types) in equilibrium integrally form a macroscopic distribution of statistically interrelated electric-$e\varphi(x)$ and chemical potential $\xi(x)$ (contained in the distribution function), as well as other thermodynamic quantities the thickness of the structure, including near the boundaries of each layer. We recall that there is no coordinate dependence of the distribution function of quasiparticles in $\mathbf{k}_i$ or energy $\varepsilon_i(\mathbf{k}_i)$ in the thickness of a homogeneous layer [8].

However, it should be taken into account that in different systems of quasiparticles, the layer thickness can be considered uniform at different distances from the boundary, and these distances depend on the physical conditions. And in a layer thin for a certain system of quasiparticles, even with homogeneous doping, its homogeneity may not be at all. If the interaction of systems in such a layer is strong, then this should also affect the distribution of fluxes of quasiparticles of other types, and with this, the distribution of thermodynamic quantities. Obviously, in complete equilibrium, the integral fluxes of charge, spin, mass and other quantities, as well as the integral fluxes of energy, entropy and other thermodynamic quantities over systems, should be zero (although the differential-elementary fluxes of the corresponding quantities are almost never equal to zero under normal conditions). This circumstance determines the system of functional equations, the joint solution of which determines the distribution of $e\varphi(x)$, $\xi(x)$ and other thermodynamic quantities in different systems over the thickness of the structure.

The coordinate dependence of the distribution function in quasiparticle systems appears in the thickness of an inhomogeneous layer due to different conditions for the propagation of fluxes through the layer thickness, associated with a change in the nature of scattering and propagation of fluxes. For the same reasons, this dependence also appears near the boundary, only the nature of the propagation of fluxes and their scattering (taking into account their exchange at the boundary) differs from a homogeneous and/or inhomogeneous layer thickness. Integral balancing of the distribution differential fluxes of quasiparticles $q_i^+(x, k_i, \Omega)$ and $q_i^-(x, k_i, \Omega)$, energy and entropy fluxes carried by them, in the entire plane-parallel layer of the finite thickness (over any of its sections $Q_j^+(x) = Q_j^-(x)$), leads to the fact that the equilibrium distribution function of charge carriers $f_o(x, k, \Omega)$, as well as the interdependent differential fluxes $q^+(x, k, \Omega)$ and $q^-(x, k, \Omega)$, depending on the coordinate and direction of propagation. And since the relaxation length of fluxes, comparable to the mean free path of charge carriers l_e, depends through the collision integral [8] on $f_o(x, k, \Omega)$ (and the distribution of differential fluxes in other systems of quasiparticles), it also has a coordinate and angular dependence $l_e(x, k, \Omega)$ in an inhomogeneous region, and in particular in the immediate vicinity of the boundary. All this leads to the fact that the symmetry in the wave vector $\mathbf{k}$ of the equilibrium distribution function inherent in the thickness of an isotropic solid layer is lost near the boundary. A similar situation occurs near the boundary for the relaxation lengths of fluxes of other kinds of quasiparticles. It is clear that the corresponding relaxation lengths in systems depend to one degree or another on the degree of interaction between the systems, both in the thickness of each layer and at its boundaries, under the physical conditions under consideration.

If the equilibrium is violated, then the given distribution of differential fluxes are modified to some extent and resultants integral (macroscopic) fluxes of a different character appear in the systems $Q_j(x) = Q_j^+(x) - Q_j^-(x) \neq 0$: fluxes of charge, energy, entropy and other thermodynamic quantities. It is clear that due to the difference in the parameters and characteristics of different systems, the integral fluxes of the corresponding quantities in them do not have to coincide. When one system of quasiparticles is considered, for example, an electronic system, under conditions of weak excitation, it is usually assumed that the temperature does not change over the thickness, i.e. its distribution is supported by equilibrium fluxes in the considered system and fluxes in other (practically equilibrium) systems of quasiparticles of the given layer. Obviously, the conditions of weak excitation, in this case, must be fulfilled both in the thickness of each layer and at its boundaries. It is also obvious that the coordinate distribution of “thermostatic” properties over different systems of quasiparticles of the structure, as well as the degree of “adiabaticity” of the layer boundaries, are largely related to the properties of the materials used in solid layers. External physical conditions exert their “thermostatic” and surface “adiabatic” influence both in the conditional equilibrium (according to Groot) case, and in the case of violation of equilibrium.

2. “Homogenous” solid-state layer: a layer within the structure and the stand-alone one

The presence of boundaries (or surfaces in a separate layer of homogeneous composition) “makes” the layer an inhomogeneous medium, since the scattering characteristics of quasiparticles at the boundaries of the layer and in its thickness are usually noticeably different. In addition, the boundary, in particular a flat one, violates the spatial symmetry of the properties (characteristics and parameters) of the layer thickness. Along with other factors, this also has a peculiar effect on the coordinate and angular dependence of the relaxation length of charge carrier fluxes at the boundary. This “spatial” circumstance must be taken into account in the mathematical formulation of the boundary-value kinetic problem of the propagation of fluxes in a solid layer, especially near its boundaries and for a thin layer as a whole. This circumstance also concerns other systems of quasiparticles, the propagation of which is described by a kinetic equation, in particular, in one or another approximation of the relaxation time. Note that in the presence of a noticeable interaction of systems as a result of scattering at the boundary, the rate of generation and transfer (removal) by differential fluxes of the total energy, entropy and other thermodynamic quantities over the systems may differ from the “volumetric” ones inherent in the layer thickness.

A structure that has several layers of physically finite thickness with different properties is a more complex inhomogeneous solid-state medium since it also has boundaries with a varied configuration and energy state. Note that the properties of the layer boundary in the structure and the boundary surface of an individual layer of similar composition can differ markedly. This is due to the difference in the final stages of the technology for growing these layers. This circumstance may be the reason for some difference in the characteristics of an individual solid layer and a layer of similar composition in the structure, along with the presence of exchange of quasiparticles in the second case.

The exchange of charge carriers and other quasiparticles between layers with different physical properties leads to the fact that the character and role of processes at the layer boundary in the structure and a separate layer of similar atomic composition and configuration turns out to be different. This affects not only the magnitude of the force fields at the boundary acting on the quasiparticles, but also the dependence of the relaxation length of the quasiparticles over the layer thickness. This difference is also influenced by the state and configuration of the boundaries of an individual layer and a layer in the structure grown on the previous layer, the second boundary of which is formed during the growth of the next layer of the structure (especially in the case of a thin layer). The indicated boundaries in these considered cases have a slightly different composition and configuration, and therefore they are characterized by correspondingly different probabilities of scattering of fluxes of quasiparticles, which affects the propagation of fluxes of charge carriers and quasiparticles of other types.

If the role of boundaries in the investigated processes of interaction of differential fluxes of charge carriers (and quasiparticles of different types in general) is essential, then it is necessary to determine as accurately as possible the dependence $l_e(x, \mathbf{k})$ near the layer boundaries (as well as $l_j(x, \mathbf{k}_j)$ for quasiparticles of other species), especially in each thin layer of the structure. As noted above, the relaxation lengths of differential fluxes directed towards and away from the boundary differ near the boundary. This is directly related to the presence of a boundary that geometrically violates the symmetry of the properties of the medium of the solid-state layer (especially towards it) and, in the general case, is the spatial section of the $\varepsilon_{ie}(\mathbf{k})$ dependences, and possibly the crystal symmetry of the solid-state layer with the corresponding consequences of this. All these factors interconnectedly affect the distribution of differential fluxes of quasiparticles, the magnitudes of the force fields [6] and the distribution of thermodynamic (statistical) quantities, primarily those that characterize the equilibrium, and through them non-equilibrium, quasiparticle distribution functions.

3. Mutual influence of force fields and the relaxation length of the fluxes nearby the boundary

The scattering of charge carriers, like other quasiparticles, at the boundary is "rigidly" fixed by its plane, in contrast to volume scattering. On boundary, it occurs inevitably, in particular, because of change of physical properties before and after boundary. For differential fluxes of charge carriers formed in the immediate vicinity of the boundary (within the region of a solid medium with a thickness $l_e(\mathbf{k})$) and directed towards it, the average distance between the acts of successive electron collisions obviously decreases in comparison with the bulk one. The closer and "more normal" the flux propagates to the boundary, the stronger the difference between $l_e(x, \mathbf{k})$ and its volumetric value.

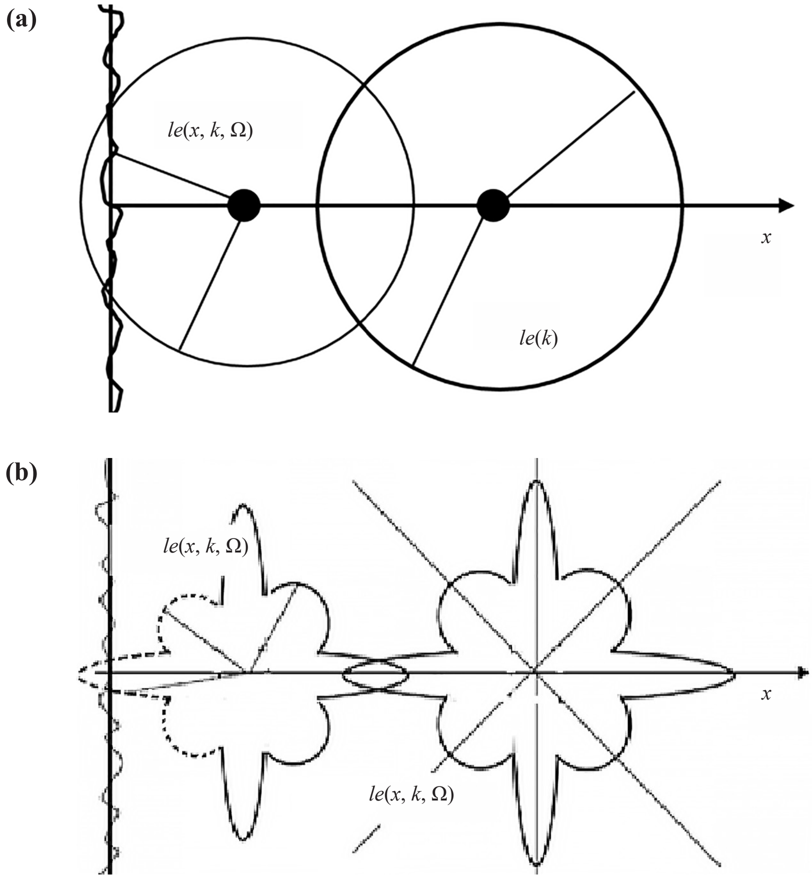

Figure 1. Explicit influence of the layer boundary on the mean free path of charge carriers and the associated relaxation length of fluxes with an isotropic distribution of properties (a) and with an anisotropic (conditional) distribution of properties (b) in a uniform thickness of a solid layer

If in the thickness of a plane-parallel solid layer with an isotropic distribution of characteristics, the relaxation length of the charge carrier flux together with the mean free path does not depend on the direction and coordinate, then their angular and coordinate dependences take place near the boundary. It is clear that the relaxation length of the fluxes of charge carriers directed from the boundary in the region of the layer located near the boundary should also depend on the properties of the boundary. Due to the presence of a relationship (through the boundary conditions [3]) of fluxes directed to the boundary, $q^{-}(x, k, \Omega)$ and all fluxes of charge carriers scattered into the same layer "from the boundary"

$q^+(x, k, \Omega)$, the configuration and state of the border implicitly influences the latter.

In the case of an anisotropic distribution of properties in a uniform thickness of a solid layer (Figure 1 (b)), the distribution of differential fluxes along the coordinate is obviously also dependent on the direction of the crystal axes with respect to the boundary normal. At the same time, the distribution of thermodynamic quantities over the thickness of a layer with an anisotropic distribution of characteristics and parameters (properties) near the boundary also depends on the direction of the crystal axes with respect to the boundary normal. Perhaps this, in some way, along with the properties of the atoms of neighboring layers, affects the formation of the boundary or surface of the solid layer.

In adjacent layers of the structure, not only the kinetic characteristics and parameters can differ, but the symmetry of the distribution of properties. This factor also affects the formation of force fields at the boundary and the distribution of thermodynamic quantities in this region of the structure. The dependence of the configuration and state of the surface of crystalline silicon (Si), as well as the distribution of the electric potential $e\varphi(x)$ near the surface, on the direction of the crystal axes with respect to the normal, have been repeatedly confirmed experimentally [19].

Along with this, the probability of scattering of differential fluxes at the boundary, which differs from the "bulk" one, as well as the exchange of charge carriers and other quasiparticles through the boundary, affect the distribution of force fields near the boundary, the relaxation length, the distribution of thermodynamic quantities and the distribution interdependent with them differential fluxes. As a result of integral functional relationships, which depend on the coordinate in an inhomogeneous medium of a solid layer and the structure as a whole, this, to some extent, affects the associated coordinate dependences of the distribution function of quasiparticles of all other types over the thickness of each plane-parallel layer of the structure. Due to these factors, the relaxation length of differential fluxes of charge carriers (and quasiparticles of other types) must be determined in a self-consistent way, together with the formation of electric and other force fields at the boundary [17, 20], taking into account the exchange of quasiparticles, both in the case of equilibrium and violation.

Obviously, for phonon fluxes, the internal force field near the boundary is the temperature gradient. This gradient in the indicated region can play a noticeable role, perhaps even the main one, as a local thermostat, which can affect the propagation of quasiparticles of different types, in particular, the propagation of charge carriers. Of course, the case of weak interaction of quasiparticles of different types in the thickness and at the boundaries of the structure is simpler than the case of their strong interaction either at the boundary and/or in the thickness of one, some or all layers of the structure.

For fluxes of charge carriers directed from the boundary, the influence of the boundary is less than for fluxes tending "to the boundary". In particular, this is noticeable even from schematic Figure 1. It can be seen that the isotropic distribution $l_e(\mathbf{k})$, and with it, the differential fluxes of charge carriers, as well as the uniform distribution of characteristics, including thermodynamic ones, inherent in the layer thickness, at the boundary is lost. Here, the relaxation length of the fluxes $l_e(x, k, \Omega)$ depends not only on the coordinate, but also on the direction (even with a very weak influence of the near-boundary force fields). Obviously, the angular indicatrix of the curve $l_e(x, k, \Omega)$ largely depends on the scattering probability $P(\mathbf{k}, \mathbf{k}_*)$ and the "sphericity" of the $l_e(x, k, \Omega)$ dependence is lost here (even in the presence of an isotropic dependence in the scattering of the charge carrier fluxes).

It is clear that the presence of the dependence $l_e(x, k, \Omega)$ at a boundary that is different from the "bulk" one should also affect the distribution of fluxes $q^+(x, k, \Omega)$ and $q^-(x, k, \Omega)$ in this region and balance, and its violation. The distribution of these fluxes, in turn, integrally forms force fields in inhomogeneous regions of the structure, including at the boundaries. The role of these fields in different circumstances can be significant or insignificant. In equilibrium, these fluxes form internal fields, which are modified in one way or another if the equilibrium is disturbed. Thus, differential fluxes of charge carriers (together with fluxes of other quasiparticles) form the resulting distribution of the electric field over the thickness of the structure, differential fluxes of phonons (together with fluxes of quasiparticles of other types) create a temperature gradient distribution (directed inward from the surface), etc. If the values of these fields are significant, then they can to some extent influence jointly the propagation of quasiparticles of all types under consideration. Excitation of systems of quasiparticles near the boundary generally changes the exchange of quasiparticles between layers. The influence of such excitation on the dependence $l_i(x, k_i, \Omega)$ turns out to be different for the corresponding fluxes of quasiparticles of different types and not the same for differential and integral fluxes directed to and from the boundary.

Note that differential phonon fluxes are scattered at the surface much stronger than in the bulk since they cannot propagate through the surface. Therefore, when the layer is heated in one way or another, the temperature gradient at the surface is directed deep into the layer, i.e. the temperature on the surface turns out to be higher than the temperature in the thickness of the layer, although it usually heats up there. This leads to the fact that at high temperatures melting begins precisely from the surface (due to the strong scattering of phonon fluxes on the surface and a large local release of energy by them with its weak removal by fluxes of quasiparticles of various types). If there is a thin oxide film on the solid layer, the melting point of which is higher than the melting point of the base material, then obviously the layer will begin to melt under this oxide film. It is this melting of layers of solid materials that are often observed in practice. This example shows the viability of the considered aspects of the kinetic theory, and also represents the scope of its application in technology.

4. Interaction of the systems of quasiparticles

Solid-state materials and structures based on them, including those in the form of plane-parallel layers, have been studied by various experimental and theoretical methods for a long time. This various long-term practice has shown that the theoretical description of a solid-state medium in equilibrium in the form of a set of non-interacting systems of quasiparticles of different physical nature, each of which is similar in properties to a specific "ideal gas", is not always satisfactory. These systems of quasiparticles (of different physical nature with very different characteristics and parameters) nevertheless interact with each other, and not equally in the bulk of the solid-state medium and at its boundaries, even in the case of the presence of homogeneity of quantum and kinetic properties in the bulk. With various disturbances in equilibrium, these systems interact in very different ways. Therefore, the mathematical description of the stationary propagation of differential fluxes of quasiparticles through the thickness of each layer of a solid structure within the framework of the kinetic theory, both in equilibrium and in case of its various violations, should be described adequately by a given boundary value problem, namely a system of interrelated kinetic equations and boundary conditions [17-18, 21]. In particular, it concerns the functioning of cascade solar cells at high insolation.

For an adequate theoretical description of the solid-state structure as a whole, it is necessary to correctly "stitch" the solution of the system of equations for all layers of the structure. In this case, the features of the propagation of quasiparticles of different types in the layers of the structure will be correctly taken into account if the distribution of thermodynamic values in the corresponding systems is determined mutually consistently.

Near the boundaries of a layer of finite physical thickness, and even more so in a thin layer, the propagation of differential fluxes of quasiparticles directed "towards the boundary" and "from the boundary", and/or in its inhomogeneous region, in each of the systems must be described by separate kinetic equations. The boundary conditions should correctly describe the relationship between differential fluxes of quasiparticles of different physical nature, including the possible exchange of quasiparticles between adjacent layers. When drawing up a system of equations and boundary conditions, it is necessary to take into account the extent to which energy and other thermodynamic quantities are exchanged between coexisting systems.

Thermodynamic quantities, which are integrally (statistically) interdependent with the distribution of differential fluxes of quasiparticles in a solid medium, are most adequately determined for the "ideal gas" system. Therefore, for each pair of kinetic equations that describe the propagation of fluxes of quasiparticles in all systems taken into account, it is desirable to correctly reduce to the corresponding description of the system of a specific "ideal gas". In this case, all the coefficients of a pair of kinetic equations in some approximation of the relaxation time, (for example, for a system of charge carriers: electric field [13], effective relaxation length of differential fluxes), as well as the distribution over the layer thickness of thermodynamic quantities in the corresponding system of quasiparticles), it is necessary to determine self-consistently (at least for the most significant systems of quasiparticles) both in equilibrium and in its violation. This especially concerns the propagation of differential fluxes near the boundaries of layers and in a thin layer of the structure as a whole, where the exchange of fluxes between its adjacent layers can play a very noticeable role. Along with correctly specified boundary conditions for differential fluxes at the boundaries of a layer of finite thickness [2], this affects the degree of reliability of the description of the physical picture both in the thickness of the considered layer and near its boundaries, including taking into account the presence of neighboring layers and exchange of fluxes of quasiparticles with different for all systems with kinetic characteristics.

If several interacting systems of quasiparticles of different kinds and types (as optical and acoustic phonons with specific properties) are considered simultaneously in a solid layer of the physically finite thickness (in a generally inhomogeneous medium), then the differential fluxes in each of them depend at least (within the framework of the ideal gas) on the wave vectors of all n given systems, i.e., $q_i(\mathbf{X}, \mathbf{K})$ where $(\mathbf{X}, \mathbf{K}) = (x_1, \mathbf{k}_1, x_2, \mathbf{k}_2, \ldots x_i, \mathbf{k}_i, \ldots x_n, \mathbf{k}_n,)$ ($i = 1, 2, \ldots, n$, and taking into account the difference in the behavior of q_i^+ and q_i^- in each system, the number of kinetic equations is equal to $2n$). The distribution functions of quasiparticles of all these systems in the general case also depend on $(\mathbf{X}, \mathbf{K})$. All systems of quasiparticles are responsible for the distribution of thermodynamic quantities over the layer thickness (in accordance with their role and distribution over the corresponding wave vectors $\mathbf{k}_i$). In this case, the simplest, physically understandable, interpretation of the results, as in the case of a simple dependence of the distributions $q_i\ (x, \mathbf{k}_i)$, turns out to be lost.

Nevertheless, if we do not take into account the effects of recycling in quasiparticle systems, using some iterative statistical averaging of the kinetic equations for the dependences $q_i^+(x, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \ldots \mathbf{k}_n)$ and $q_i^-(x, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \ldots \mathbf{k}_n)$ the physical picture can be reduced to "simple" and understandable distributions of the fluxes $q_i^+(x, \mathbf{k}_i)$ and $q_i^-(x, \mathbf{k}_i)$. Without recycling [22], the fluxes in the collision integral are scattered locally, that is, they depend on one coordinate x. After such averaging, the interaction of different systems of quasiparticles will in some way be mutually coordinated and taken into account, and the systems can formally be considered mutually independent. It is in such systems that the distribution of thermodynamic quantities is most adequately determined. It is clear that under different conditions, due to the difference in the physical properties of these systems, the coordinate distribution of thermodynamic quantities will not coincide in all of them (for example, as the specific temperature of "hot" electrons).

5. Justification of the need for studying joint propagation of quasiparticles in solids

Even without solving the kinetic boundary value problem, using the general form of the collision integral [8], it is easy to find the relationship between the equilibrium distribution function of electrons $f_o(\mathbf{k})$ in the thickness of a homogeneous solid layer with the transition probability $W(k, k')$ from a state with a wave vector k to a state k' and the probability $W(k', k)$ of the reverse transition from k' to k-state:

$$f_o(k) = \left\{1 + \left[\sum\nolimits_{k'} W(k,k')(1 - f_o(k')) \,/\, \sum\nolimits_{k'} W(k',k) f_o(k')\right]\right\}^{-1} \tag{1}$$

The elementary formulated events $A(\mathbf{k} \to \mathbf{k}')$ and $A'(\mathbf{k}' \to \mathbf{k})$ are quite complex, and even mysterious, in terms of their implementation in specific conditions. The mysteriousness of these transition probabilities is due to the lack of instructions in the kinetic theory to specify the various mechanisms of the transition (and their role) from the $\mathbf{k}'$ state to the $\mathbf{k}$ state and back. It is clear that the transitions $\mathbf{k}' \to \mathbf{k}$ (as some event A') and $\mathbf{k} \to \mathbf{k}'$ can be carried out in various physical ways [8]. As shown above, these transitions are associated with the propagation and scattering of fluxes not only of a system of electrons, but also of systems of quasiparticles of other types, if they actively interact with it [17-18]. In this case, a redistribution of differential fluxes of energy, entropy and integral fluxes thermodynamic quantities between the systems occurs. It is clear else that some transition mechanisms are more probable, and some less probable; moreover, this difference is not the same for a homogeneous layer and near the layer boundary or in its other inhomogeneous region.

This remark concerns not only transitions within any one system of quasiparticles, but also transitions due to the presence of systems of quasiparticles of other types. If not all, then at least the most significant interacting systems are necessary for the correct description of the propagation of the total fluxes of energy, entropy and other thermodynamic quantities that take place in the solid medium of the layer under consideration. When one more system of quasiparticles of a certain kind (or type) is added to the kinetic description of the propagation of fluxes, the probabilities of transitions, for example, from $\mathbf{k}'$ to the $\mathbf{k}$-state and back should be self-consistently redefined.

If the redistribution of thermodynamic quantities over the systems is not taken into account, then the losses of energy and other quantities in the analyzed one system of quasiparticles drop out of consideration and are lost without a trace. In reality, the systems interact over the entire thickness of the layer and its can, at least partially (if there are fluxes out of the layer and the structure), return these losses to each other. Precisely because of the complete account of the mutual influence of different systems of quasiparticles on each other, each solid-state system exists in a (conditional) equilibrium state. Note that the external physical medium acts directly on some systems of quasiparticles of the solid layer and the structure as completely stronger, on others weaker. But due to the presence of interaction between systems, it indirectly affects other systems of quasiparticles. If the state of the external physical medium due to some external circumstances changes rather slowly in comparison with the processes of formation of thermodynamic quantities in all systems of quasiparticles of a solid matter, then the thermodynamic quantities will adequately describe the physical picture in a solid matter. The thermodynamic influence of all systems of solid-state layers on the external medium (usual locally) is similarly diverse and specific. The functioning of the powerful solid-state laser is a convincing example, proving this statement.

The considered losses in one of the systems of a thick layer are mainly redistributed over different systems of quasiparticles, and only some of them, which occurred mainly near the boundary, leave the layer. In a layer that is thin for the propagation of quasiparticle fluxes of some (or all) systems, the situation can change significantly. The propagation of quasiparticles in a thin layer acquires the features of ballistic motion. In this case, the usual thermodynamic characteristics of such systems of quasiparticles are not quite adequate. In this case, the characteristics of the integral fluxes of quasiparticles change little over the thickness of the layer, and the redistribution of losses is largely due to the mechanisms of scattering of differential fluxes at the boundaries of the layer, as well as the intensity of exchange of fluxes of quasiparticles.

In approximately the same way, the external medium (a general thermostat for the structure) acts with its specific fluxes, corresponding to external conditions, on systems of quasiparticles of solid-state layers of the structure through its surface. Moreover, for some external fluxes, in particular for photon fluxes (for example, from the infrared region of the spectrum), the solid-state layers of the structure can be thin. However, the fluxes of atoms of the external medium under normal conditions practically do not enter the solid-state matter, although they exchange their energy, mainly with the phonon system, as a result of their reflection from the hesitate boundary.

The equilibrium in the considered system as a whole corresponds to the given physical conditions and is associated with the conditional equilibrium of all other systems of the solid-state layer. Here it should be taken into account that the distance from the boundary, at which its significant influence ends and the homogeneous layer thickness can indeed be considered uniform, for various systems of quasiparticles can differ markedly. Under various physical circumstances, this difference in the indicated distances (the dimensions of a region near the boundary that is inhomogeneous for a certain system) is not necessarily preserved, i.e. they can change in each system depending on external and internal conditions. These circumstances significantly complicate the physical picture that occurs in a solid-state structure. Moreover, this, in turn, complicates the physical interpretation of various experimental data.

In a homogeneous medium, the equilibrium in systems is everywhere the same in its volume, although it depends on the physical properties of the medium, distributed uniformly. In an inhomogeneous medium, including a homogeneous layer of physically finite thickness, the equilibrium in systems depends not only on the properties of the medium, but also on the nature of the inhomogeneity in the layer. And the nature of the inhomogeneity of the properties of the medium can be very diverse. Therefore, in the latter case, the equilibrium, in contrast to the usual equilibrium in a homogeneous medium, turns out to be conditional. It essentially depends on the conditions for the propagation of quasiparticle fluxes in an inhomogeneous region of the medium, in particular, the medium of a solid layer. In principle, ordinary equilibrium in a homogeneous solid medium can be regarded as a special case of “conditional equilibrium” when there is no inhomogeneity in the medium. Thus it is not necessary to forget that the property of homogeneity depends on the viewed gauge.

Near the boundary, due to its specific properties and possible exchange processes of quasiparticles, as well as due to more frequent than in the layer thickness, scattering acts concentrated (localized) at the boundary, the nature of the “stationarity” of random physical quantities changes and their belonging to the form that is present in the thickness of the layer can be lost. This region is “transitional”, in it the probabilities of various processes and the nature of the exchange, quasi-momenta and quantities associated with the propagation of quasiparticle fluxes change significantly. The averaging of the values “overtime” and “overstates” near the boundary and in the thickness of the layer may not coincide. The degree of loss of the ergodicity property in some or all of the quasiparticle systems can be noticeable here.

Comparing expression (1) with the usual Fermi-Dirac function, which describes the distribution of electrons in a homogeneous medium in equilibrium, we obtain

$$\exp\left(\frac{\varepsilon_e(\mathbf{k})-\xi_0}{k_0T_0}\right)=\left[\sum\nolimits_{k'}W(k,k')(1-f_o(k'))/\sum\nolimits_{k'}W(k',k)f_o(k')\right] \tag{2}$$

Here $\varepsilon_e(\mathbf{k})$ is the dispersion law of electrons, ξ_o is the chemical potential in equilibrium, and k_oT_o is the thermal energy of electrons. For an adequate understanding of the mechanisms of formation of thermodynamic quantities in the left and right sides of expressions (1) and (2), the transition probabilities $W(\mathbf{k}, \mathbf{k'})$ and $W(\mathbf{k'}, \mathbf{k})$ must explicitly contain terms describing the ways of changing wave vectors and in other systems of quasiparticles. If in expression (2) we use the “principle of detailed balance” without disclosing the essence of the probabilities W, then its left side is identically equal to the right side. Obviously, this solution to the functional equation (1) or (2) is not the only possible one. Therefore, this principle should be regarded as the most probable for a state of equilibrium. This principle can also be preserved near the border, although the value of the “most probable” of its fulfillment here is most likely already different, i.e. its reliability decreases, including due to the influence of the neighboring medium-a solid layer.

In an inhomogeneous region of a plane-parallel layer, in particular, in the immediate vicinity of the boundary, both transition probabilities W (associated with fluxes through the scattering cross-section) depend on the coordinate in a complex manner, since the conditions for propagation and scattering of differential and integral fluxes of electrons (as well as other quasiparticles) vary in thickness layer. Therefore, the exponent in the left and right sides of expression (2) (in the function $f_o(\mathbf{k})$) should also depend on the coordinate.

Note that the inhomogeneity of a plane-parallel layer over its thickness can have a different character. For example, the atomic composition or the degree of alloying, the concentration of defects, etc., or both together can vary in thickness. It follows that, in the general case, the coordinate dependence of the exponent is due to the character of the dependences $W_{ij}(x, ..., \mathbf{k}_i, ... \mathbf{k}_j, ...)$, inherent in the considered an inhomogeneous solid layer (or, as a special case, its homogeneous thickness).

Thermodynamic quantities in each system of a physically different nature are expressed in the most adequate way if the system can be correctly defined as a kind of “ideal gas”. Thus, the coordinate dependence of the equilibrium distribution function of electrons in a plane-parallel solid layer $f_o(x, \mathbf{k})$ with allowance for the scattering of differential fluxes of quasiparticles on each other, in general, is also due to the same dependences $W_{ej}(x, ..., \mathbf{k}_e, \dots \mathbf{k}_j, ...)$ and $W_{je}(x, ..., \mathbf{k}_e, \dots \mathbf{k}_j, \dots)$, averaged over all other $\mathbf{k}_j$. Consequently, in the general case, the distribution function of electrons in an inhomogeneous solid layer in equilibrium can depend on the coordinate manifoldly:

$$f_o(x,\mathbf{k})=\left\{1+\exp\left(\frac{\varepsilon(x,\mathbf{k})-e\varphi_0(x)-\xi_0(x)}{k_0T_{e0}(x)}\right)\right\}^{-1} \tag{3}$$

In this case, the right part of the kinetic equation in balance has a bulkier (difficult) view. If the atomic composition does not change over the layer thickness, then it is usually assumed that the dispersion law $\varepsilon_e(\mathbf{k})$ does not depend on the coordinate and the temperature of the electron system is also constant.

In expression (2) we can determine the sums with probabilities W through the differential fluxes of not only charge carriers, but also quasiparticles of other types propagating and scattering in the medium of a solid-state layer [23-24], which play an appreciable role in the given physical conditions. If to take the logarithm of this expression, then the dependence of the combination of distributions of thermodynamic quantities on the distribution of differential fluxes of quasiparticles of different types will become apparent. Although the coordinate dependence of the combination of distributions of thermodynamic quantities on the probabilities W is logarithmic, i.e. weak, nevertheless, it is still there.

You can simply take into account in the above way the influence of the interaction of a system of charge carriers with systems of other quasiparticles and find the distribution of thermodynamic quantities from simpler statistical (integral) functional expressions that formally correspond to a specific system of particles of an “ideal gas”. Recall that when determining thermodynamic quantities in an inhomogeneous region of a layer, including at the boundary, it is necessary to take into account the propagation and dispersion of differential fluxes of two classes, namely, those directed to and from the boundary, separately. However, directly at the border, the circumstances of the formation of thermodynamic quantities turn out to be more complicated.

In the case of studying the equilibrium state of the phonons system in an inhomogeneous solid-state medium, the distribution function in the exponential contains only one thermodynamic quantity, namely, temperature [21, 25]. The presence at the boundary, by analogy with [13], of a force field for phonons-a temperature gradient (possibly weak), means the presence of a coordinate dependence of the temperature in the considered region. Due to the interaction between systems, this circumstance affects not only the distribution of phonon fluxes in an inhomogeneous region (including at the boundary), but also, to some extent, the distribution of fluxes and thermodynamic quantities in other systems of quasiparticles. Although the collision integral for quasiparticles-bosons, which are phonons of all branches and types (as well as photons of different polarizations), is somewhat different from the "fermionic" one, nevertheless, it is easy to obtain for these quasiparticles the relationship between their distribution and the scattering probabilities (of these quasiparticles) $W(k, k')$ and $W(k', k)$ [24]. A form of this expression will be in many respects similar to expression (1-2).

6. Influence of the boundary on the thermodynamic values distribution

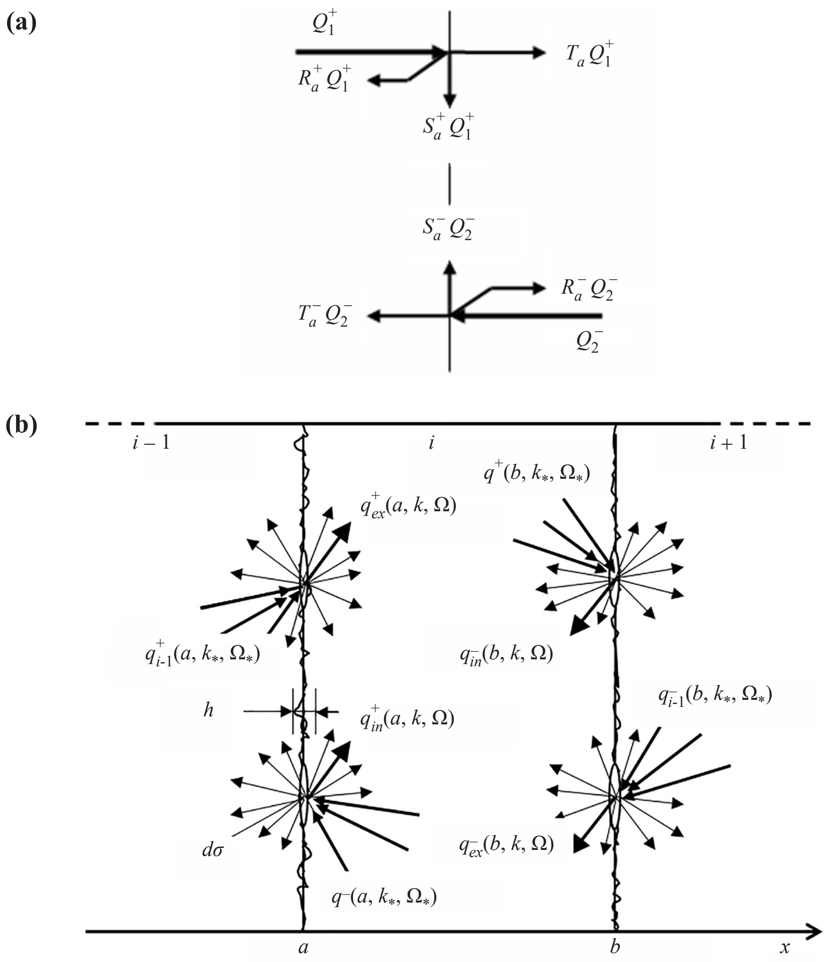

Figure 2. Scattering of integral (a) and differential (b) fluxes of charge carriers at the interface between solid layers with different quantum and kinetic characteristics

Let us consider the general physical picture occurring at the interface between media and charge carriers. The (integral) fluxes of charge carriers $Q_1^+(a)$ and $Q_2^-(a)$, consisting of different sets of differential fluxes $q_1^+(a, k, \Omega)$ or $q_2^-(a, k, \Omega)$. In the general case, some part of R, of all carrier fluxes incident from one of the sides, is reflected, part of T passes through it, and some part of S is lost on it. In this case, it is obvious that the condition $R + T + S = 1$ must be satisfied on each side of the border. Integral fluxes directed to the left of the border, $Q_1^-(a) = R_1^+Q_1^+(a) + T_2^-Q_2^-(a)$, and directed to the right of it, $Q_2^+(a) = R_2^-Q_2^-(a) + T_1^+Q_1^+(a)$, are formed taking into account the possible propagation of differential fluxes from an adjacent (adjacent) layer (see Figure 2a).

Note that in neighboring layers the quantum and kinetic characteristics, through which the corresponding differential fluxes are determined (see below), can differ significantly. Therefore, the resulting integral flux $Q(a) = Q^+(a) - Q^-(a)$ in the layer to the left of the boundary and the right of it has a different total composition of differential fluxes. In this case, in the indicated aggregates, the exchange of charge carriers across the boundary, which has their own velocity distributions, is correctly taken into account.

In accordance with the formation of integral fluxes, it is possible to describe in detail the probabilistic "fate" of each differential flux $q_1^+(a, k, \Omega)$ and $q_2^-(a, k, \Omega)$ falling on the boundary after scattering. To do this, you need to know the probabilities of scattering (forward and backward) of all differential fluxes incident on the boundary. By collecting all the contributions from each flux scattered by the boundary to a certain, arbitrarily selected, differential flux in the layer under consideration (see Figure 2b), It is not difficult to obtain the boundary condition for the corresponding kinetic equation. A similar physical picture, but with specific scattering probabilities and, accordingly, coefficients, takes place at the boundary and for fluxes of other kinds of quasiparticles.

In the thickness of the plane-parallel layer, the integral fluxes of charge carriers are equal

$$Q^+(x) = \int\limits_{V_B^+} q^+(x,k,\Omega^+)\cos\theta\, k^2 dk\, d\Omega^+$$

$$Q^-(x) = \int\limits_{V_B^-} q^-(x,k,\Omega^-)\cos\theta\, k^2 dk\, d\Omega^- \tag{4}$$

where V_B^+ is the region of the Wigner-Seitz cell (the first Brillouin zone in symmetric form) with a positive projection of the wave vector k, and V_B^- is the region of the cell with a negative projection k for the layer under consideration, the solid angle $\Omega = \Omega\ (\theta, \varphi)$ indicates the direction of propagation of this differential flow, $d\Omega = \sin\theta d\theta d\varphi$, (hereinafter $|\cos\theta| = \mu$). The sets of differential fluxes (two "classes") corresponding to this separation of the integral fluxes of charge carriers in the thickness of the layer are equal to

$$q^+(x,k,\Omega^+) = 2v(k)f(x,k,\Omega^+)/(2\pi)^3 \text{ and } q^-(x,k,\Omega^-) = 2v(k)f(x,k,\Omega^-)/(2\pi)^3. \tag{5}$$

These fluxes propagate in an isotropic medium in the direction of the vector k, which belongs to the right Ω^+ or left Ω-part of the Wigner-Seitz cell inherent in the crystalline layer under consideration. Since the belonging of the differential flow to the direction of propagation in Ω^+ or Ω^- is directly in the designation of the corresponding flux, then in its argument the superscript at Ω will not be used to simplify the notation. The velocity of a quasiparticle in the fluxes is determined by the corresponding dispersion law $\varepsilon(\mathbf{k})$, namely $\mathbf{v}(\mathbf{k}) = \hbar^{-1}\mathrm{grad}\ \varepsilon(\mathbf{k})$ [4]. In an isotropic medium, the direction of the vector $\mathbf{v}(\mathbf{k})$ coincides with the direction of $\mathbf{k}$, as well as the differential flux itself.

However, at the border located for example at $x = a$ (see Figure 2b), in contrast to the thickness of a homogeneous solid layer, as shown above, there are some peculiarities in the definition of $Q^+(a)$ and $Q^-(a)$. In particular, the differential carrier fluxes $q^+(x, k, \Omega)$ and $q^-(x, k, \Omega)$ in adjacent layers are due to different dependencies of the velocities $\mathbf{v}_{i-1}(\mathbf{k}_{i-1})$ and $\mathbf{v}_i(\mathbf{k}_i)$, as well as the effective masses of the carriers, charge in adjacent layers, in accordance with the dispersion laws $\varepsilon_{i-1}(\mathbf{k}_{i-1})$ and $\varepsilon_i(\mathbf{k}_i)$ in these layers of the structure. This must be taken into account, since $\hbar\mathbf{k}_{i-1} = \mathbf{p}_{i-1} = m_{i-1}\mathbf{v}_{i-1}$ and $\hbar\mathbf{k}_i = \mathbf{p}_i = m_i\mathbf{v}_i$. In addition, the V_B^+-region is the Wigner-Seitz cell region for the adjacent layer $(i - 1)$ with a positive projection of the wave vector k, and V_{Bi}^- is the cell region with a negative projection $\mathbf{k}$ already for the considered layer i. Due to the possible difference in the symmetry of the crystal lattice of neighboring layers, these regions may not coincide in their structure. The question of the specific form of these parts of the cells and the structure of the energy zones in the border region should be solved within the framework of quantum mechanics.

The resulting integral flux of charge carriers in both cases, both at the boundary of the structure and in the thickness of any of its layers, is $Q(x) = Q^{+}(x) - Q^{-}(x)$. If we do not consider the fluxes of quasiparticles (systems) of other types, with which fluxes of energy, entropy, etc. are also exchanged at the boundary. (i.e., when the fluxes of charge carriers are scattered, fluxes of phonons, photons, etc. are disturbed or excited), then the losses $S_a^{+}Q_1^{+}$ and $S_a^{-}Q_2^{-}$ in the system of charge carriers are then simply lost. The more significant systems (fluxes) of quasiparticles are taken into account in the mathematical model of the propagation of quasiparticles both at the boundary and in the thickness of the solid layer, the more accurate and adequate the model will be. However, the mathematical complexity increases markedly. Obviously, there needs to be a certain balance between the adequacy of the theoretical description and the increase in mathematical complexity.

It is clear that differential fluxes of different types of quasiparticles actually fall on the boundary, also from both sides of it. If in Figure 2b to imagine the presence of incident and scattered fluxes of quasiparticles of other kinds than the drawn incident and scattered differential fluxes of charge carriers, then the formally schematic picture remains the same. However, physically it will become richer and more adequate, as well as mathematically more complex. In adjacent layers, all these differential fluxes also have different quantum and kinetic characteristics for each of the systems, in particular, the dispersion laws $\varepsilon_i(k_i)$ or $\hbar\omega_j(\mathbf{k}_j)$. Therefore, at the boundary, their integral fluxes, determined according to the rules similar to those for the integral fluxes of charge carriers, also have specific features.

Each flux incident on the boundary with a certain probability P_a is scattered on it and makes the corresponding contributions to each (any) scattered flux $q(a, k, \Omega)$ both inside the layer and in the general case outside of it. In this case, the losses of thermodynamic quantities associated with the losses of the integral fluxes $S_{ai}^{+}Q_{1i}^{+}$ and $S_{ai}^{-}Q_{2i}^{-}$, which occur at the boundary, are redistributed over all other systems of quasiparticles and their fluxes in both adjacent layers. This consideration is especially important if the losses in the integral fluxes at the boundary are large and the interaction of the systems is significant.

By virtue of the above, the integral boundary condition for the scattering of charge carrier fluxes on the left boundary of the considered plane-parallel solid-state layer (without taking into account the presence of other systems of quasiparticles) for the stationary kinetic equation can be written in the following form [13]:

$$q_i^{+}(a,k,\Omega)\mu = \int\limits_{V_{Bi-1}^{+}} P_a^{+}(k,\Omega,k_*,\Omega_*)q_{i-1}^{+}(a,k_*,\Omega_*)\mu_* k_*^2 dk_* d\Omega_* + \int\limits_{V_{Bi}^{-}} P_a^{-}(k,\Omega,k_*,\Omega_*)q_i^{-}(a,k_*,\Omega_*)\mu_* k_*^2 dk_* d\Omega_* \tag{6}$$

Here V_{Bi-1}^{+} is the area of the Wigner-Seitz cell (Brillouin zone) at the boundary for layer $(i - 1)$ with a positive projection of the wave vector k, and V_{Bi}^{-} is the area of the cell with negative projection k already for the considered layer i. The flux $q^{+}(a, k, \Omega)$-is the density of the differential flux of charge carriers with the modulus of the wave vector k, propagating from the boundary $x = a$ in the direction near $\Omega = \Omega(\theta, \varphi)$, into the thickness of the layer under consideration, $\mu = |\cos\theta|$, $d\Omega = \sin\theta d\theta d\varphi$. A similar condition can be written for the right boundary of the layer under consideration.

The first term in (6) describes the contribution to the flux $q_i^{+}(a, k, \Omega)$ from the scattering of all fluxes incident on the left boundary of layer i under consideration outside of it. The second term gives the contribution from all flows falling on the same boundary from the inside. To simplify the notation, by virtue of integration, the wave vector $\mathbf{k} \geq (k, \Omega(\theta, \varphi))$ of the incident fluxes do not have here the indices belonging to the corresponding solid layer.

If we take into account the differential fluxes of quasiparticles of other types, which also actually fall on the boundary from two sides and scatter on it, then in expression (6) it is necessary to add (take into account) the pairs of integral terms of a similar type corresponding to the systems [2]. In the latter case, the boundary or surface is characterized by a set of scattering probabilities P_{ij} of fluxes of quasiparticles of different types.

Similarly, there is an integral relationship between the fluxes $q^{-}(b, k, \Omega)$ and $q^{+}(b, k, \Omega)$ on the right boundary of the layer under consideration [13]. However, the integration, in this case, is carried out over the regions V_{Bi}^{+} and V_{Bi+1}^{-}. Integral boundary conditions of the form (6) connect at the boundary not only fluxes, for example, $q^{-}(b, k, \Omega)$ and

$q^+(b, k, \Omega)$ in a layer, with each other, but also agree on them with flows in neighboring layers having own physical characteristics. To obtain a general solution over the entire thickness of a plane-parallel solid structure, it is necessary to "stitch" the solutions of the kinetic equation (or a system of equations for the joint propagation of quasiparticles of different types) at all boundaries of the structure in accordance with the boundary conditions.

In the general case, it should be borne in mind that all differential fluxes $q_i^+(x, \mathbf{k}_i)$ and $q_i^-(x, \mathbf{k}_i)$ that appear in the theoretical description specifically carry with them across the boundary not only charge (if the quasiparticle has one), but also specific for systems of adjacent layers, energy, entropy, and other quantities. Due to this, due to a special-"boundary", method of formation of flows, for example, $q^+(a, k, \Omega)$ and $q^-(a, k, \Omega)$ in accordance with expression (6), at the considered boundary of the layer, (as well as at other boundaries of the structure), the usual thermodynamic quantities (characteristics), as for a homogeneous medium, are not entirely appropriate here.

The very formation of thermodynamic quantities in this region occurs specifically, mainly due to "one-act" scattering of fluxes at the boundary, albeit probabilistic. Here, in the case of the exchange of fluxes of charge carriers, a kind of mixing of differential fluxes takes place (see Figure 2a.) With quantum characteristics different on both sides of the boundary, in particular, with different dispersion laws $\varepsilon_1(\mathbf{k})$ and $\varepsilon_2(\mathbf{k})$ and dependences of the velocities $\mathbf{v}_1(k)$ and $\mathbf{v}_2(k)$, as well as effective masses and specific coordinate-dependent regions of integration-peculiar parts of the Wigner-Seitz cells. This mixing of fluxes distributed over k and carried by streams of energy, entropy, etc., also depends on the properties of the boundary itself. These properties can differ significantly from the "bulk" ones, which are provided by various scattering mechanisms and, in general, by "multi-act" distributed mixing in the thickness of the layer. In contrast to the propagation of differential flows in an inhomogeneous stratum of a solid layer, these statements are specific precisely for the propagation of flows across the boundary.

Solutions of the boundary-value kinetic problem in each layer of the structure-a system of equations for a pair of differential fluxes of quasiparticles of the most significant kinds $q_i^+(x, \mathbf{k}_i)$ and $q_i^-(x, \mathbf{k}_i)$, must be correctly "stitched" in accordance with the boundary conditions at each boundary of the structure. In this case, it turns out that various differential fluxes of quasiparticles and the energy, entropy, etc. carried by them from neighboring layers affect, in one way or another, the propagation of similar fluxes in each layer under consideration. They jointly form the distribution of thermodynamic quantities in systems of quasiparticles, in the general case: electric $e\varphi(x)$) and chemical $\xi(x)$ potential, as well as temperature $T(x)$, over the entire thickness of the structure. Therefore, in each layer of the structure, the self-consistency of the solution of the kinetic boundary value problem in terms of the coefficients of the system of kinetic equations should also be ensured taking into account the boundary conditions and the influence of the propagation of fluxes of different systems of quasiparticles on the formation of distributions of thermodynamic quantities in these systems. In such a decision, the specific physical properties of all layers of the structure and their influence on each other both in equilibrium and when it is violated are adequately taken into account.

The indicated self-consistent solution will correctly describe the physical picture, including the change in thermodynamic quantities in all systems, over the thickness of the solid-state structure, both in equilibrium and when it is violated. It is clear that the heterogeneity of the structure, due to the difference in the properties of its layers and the presence of boundaries, has a peculiar effect on the formation of the distribution of thermodynamic quantities near each boundary of the structure and its surface. In this case, at each boundary and in the immediate vicinity of it, it is necessary to take into account the peculiarities of the formation of the thermodynamic quantities of all systems, i.e. introduce a more adequate specific description of quasiparticle systems. In an inhomogeneous region located in the thickness of the layer, for example, in the region of the *p-n*-junction, such a specific description can also be more adequate than the usual one.

The energy flux density carried by charge carriers (see, for example, [26-27]) in the thickness of a plane-parallel solid-state layer, taking into account expressions (5), in the general case, can be written in the form

$$Q_\varepsilon(x) = \int\limits_{V_{B1}^+(x)} \left[\varepsilon(x,k) - \xi(x)\right] q^+(x,k,\Omega)\, \mu k^2 dk d\Omega \;-\; \int\limits_{V_{Bi}^-(x)} \left[\varepsilon(x,k) - \xi(x)\right] q^-(x,k,\Omega)\, \mu k^2 dk d\Omega) = Q_\varepsilon^+(x) - Q_\varepsilon^-(x) \qquad (7)$$

It is necessary to use this expression directly at the boundary carefully, taking into account the difference in the properties of neighboring layers, as in the formation of the integral flux of entropy and other thermodynamic quantities. It is clear that the structure and state of the boundary affect not only the scattering probabilities of differential fluxes of quasiparticles, but also the regions of integration.

In equilibrium in an isotropic homogeneous mass, the coordinate dependence in expression (7) is completely absent. Far from the boundaries $q^+(x, k, \Omega) = q^-(x, k, \Omega) = q(k, \Omega)$ and the non-zero energy fluxes Q_ε^+ and Q_ε^- (and other quantities) balance each other everywhere, as well as the integral fluxes of quasiparticles themselves. But in an inhomogeneous region of the layer thickness or at the layer boundary (both an individual and a layer in the structure), in the general case, the dependences of the differential fluxes of charge carriers are not the same and $q^+(x, k, \Omega) \neq q^-(x, k, \Omega)$. Nevertheless, in equilibrium, the resulting energy flux should be zero, and the integral energy fluxes may depend on the coordinate $Q_\varepsilon^+(x) = Q_\varepsilon^-(x)$.

This means that the exchange of energy in the inhomogeneous thickness of the layer, with other systems of quasiparticles, does not occur in the same way over the thickness of the layer. Due to this, at least some thermodynamic characteristics in the distribution function of carriers (and in their differential fluxes, the wave vector of which belongs to the cell region V_B^+ or V_B^-), in some way not in the same way depending on the coordinate. These circumstances lead to the fact that in other systems of quasiparticles the thermodynamic characteristics in an inhomogeneous region depend on the coordinate, possibly weakly. Compared to a separate layer, at the boundary of adjacent layers of a solid-state structure, the situation is complicated by the exchange of fluxes of quasiparticles between the layers, although the general essence remains the same if we take into account the difference in quantum and kinetic characteristics in adjacent layers of the structure.

If we denote $Q_{\varepsilon kin}^+$ and $Q_{\varepsilon kin}^-$ corresponding to the kinetic energy flux densities in expression (7), then, taking into account (4), in the inhomogeneous region of the solid layer and near the boundary, among other things, we can determine the chemical potential of the integral fluxes of charge carriers $Q^+(x)$ and $Q^-(x)$:

$$\xi^+(x) = \left(Q_\varepsilon^+(x) - Q_{\varepsilon kin}^+(x)\right) \Big/ Q_\varepsilon^+(x) \text{ and } \xi^-(x) = \left(Q_\varepsilon^-(x) - Q_{\varepsilon kin}^-(x)\right) \Big/ Q_\varepsilon^-(x). \tag{8}$$

This definition of the chemical potentials of flows in equilibrium does not contradict its definition in a homogeneous mass. In this case $\xi^+(x) = \xi^-(x) = \xi$. Moreover, such a definition of a pair of chemical potentials of a pair of integral fluxes is also convenient to use when equilibrium is violated, when the dependences of differential fluxes in the general case differ not only in the dependences of differential fluxes, $q^+(x, k, \Omega) \neq q^-(x, k, \Omega)$, but also the dependences of their integral fluxes $Q^+(x) \neq Q^-(x)$. In the latter case, there are coordinate-dependent resulting integral fluxes of not only energy, but also entropy and other thermodynamic quantities (in different systems of quasiparticles, if there is a noticeable interaction).

It is clear that under some physical (external and/or internal) conditions for the functioning of a solid-state structure, it is possible that the coordinate dependence of some thermodynamic quantities (characteristics) in quasiparticle systems will turn out to be insignificant. In other operating conditions of the structure, as practice shows, this dependence must be taken into account. In both versions, assessing the situation requires an adequate understanding of the physical picture that occurs with the fluxes of quasiparticles in their different systems, not only at the boundaries of a solid structure, but also in the thickness of each of its layers. In the second case, it will be difficult to purposefully optimize the structure of one or another solid-state device, which consists of several solid-state layers with different characteristics, without taking into account the coordinate changes in thermodynamic quantities over the thickness of the structure. As a result, due to an incomplete understanding of the physical picture, the development or optimization of the device can be time-consuming and very expensive.

In an inhomogeneous region of the layer, as well as when the equilibrium is violated in different ways, a successful variant of a more adequate description (especially at the boundary) can be a similar operation along with the density of the integral fluxes of quasiparticles $Q_i^+(x)$ and $Q_i^-(x)$ of different systems, the use of the densities caused by integral energy fluxes $Q_{\varepsilon i}^+(x)$ and $Q_{\varepsilon i}^-(x)$, entropy $Q_{Si}^+(x)$ and $Q_{Si}^-(x)$ and other thermodynamic quantities. With the help of the latter, it is easy to determine the thermodynamic characteristics of directly integral fluxes of quasiparticles of the corresponding types, for example, phonons crossing the boundary from different sides. Of course, in this case, one should take into account the specificity in the distribution of the shares of T_jQ_j, R_jQ_j and of the corresponding valueson both sides of the border. With their help, it is not difficult to correctly determine the temperature of the integral flux directed to and from the boundary in each layer of the structure, if the distributions of differential fluxes $q_j^+(x, k_j, \Omega)$ and

$q_j^-(x, k_j, \Omega)$ over all layers of the structure are determined correctly.

The determination of the temperature of the (integral) particle flux was introduced in different works (see, for example, [9]). Similarly, one can determine the chemical potential of significant integral fluxes of quasiparticles of different types. However, the correct definition of a pair of thermodynamic values of fluxes in an inhomogeneous region corresponding to a pair of integral fluxes of quasiparticles $Q_i^+(x)$ and $Q_i^-(x)$ has not been introduced earlier. Such a theoretical description of the thermodynamic characteristics of a medium is also more appropriate when the proportion of ballistic propagation of quasiparticle fluxes of any or all types of quasiparticles in a solid layer noticeably prevails over "diffuse"-multi-act scattering during flow propagation. In this case, the integral fluxes of energy, entropy and other quantities carried by the corresponding fluxes of quasiparticles also turn out to be (at least partially) ballistic.

At the boundary, and even in an inhomogeneous region in the thickness of the layer, the indicated thermodynamic values of the density of the corresponding different integral fluxes of quasiparticles $Q_i^+(x)$ and $Q_i^-(x)$ in opposite directions along the normal to the boundary describe the physical picture more correctly than simply the usual coordinate distribution of thermodynamic quantities. Obviously, in a homogeneous region of the layer thickness, due to the symmetry of the isotropic medium (and the distribution of differential fluxes of quasiparticles) in equilibrium, the indicated thermodynamic values of the integral fluxes $Q_i^+(x)$ and $Q_i^-(x)$ in different systems are the same, and the integral fluxes of quasiparticles themselves balance each other. In this case, this description, like the usual distribution of thermodynamic quantities along the coordinate, in the thickness of the layer also turns out to be completely adequate (see expression (7)).

Note that energy and entropy are additive thermodynamic quantities. Therefore, the resulting fluxes of energy and entropy in the solid-state layer are the sum of the corresponding differential fluxes, which form integral fluxes over the systems of quasiparticles under consideration. In equilibrium, the resulting fluxes, in particular fluxes of energy density $Q_\varepsilon(x) = \Sigma\,(Q_{\varepsilon i}^+(x) - Q_{\varepsilon i}^-(x))$, should be absent. This condition is fully satisfied in the absence of resultant energy fluxes in all formally independent systems of quasiparticles of the solid layer.

Obviously, the temperature of the integral flux of quasiparticles ($Q_i^+(x)$ or $Q_i^-(x)$) of different kinds can be determined through the ratio of the corresponding integral fluxes of energy to the integral flux of entropy. A pair of chemical potentials of integral fluxes of quasiparticles of different systems is determined (similarly to expression (8)) by the ratio of the corresponding integral flux of energy to this integral flux of quasiparticles in the same direction. In this case, the mathematical description of the picture occurring in a solid structure in the extended range of changes in external and/or internal physical conditions will be more adequate. Of course, differential fluxes of quasiparticles of different types, which form all integral fluxes, should be determined self-consistently, not only by the coefficients of the system of kinetic equations, but also by the coordinate distribution of thermodynamic quantities found taking into account the integral boundary conditions and the corresponding renormalization of the scattering probabilities when included in the theoretical description of new systems of quasiparticles as described above.

Mathematical expressions that jointly describe the indicated conditions for the equality of integral fluxes along the coordinate of a structure that is inhomogeneous as a whole can serve as functional expressions for the correctly self-consistent determination of the initial distribution of thermodynamic quantities over homogeneous regions in the layers of the structure in equilibrium in all systems of quasiparticles considered jointly. Due to this, any conditional equilibrium in the structure corresponding to stationary external conditions can be characterized by a certain conditional equilibrium of the considered integral fluxes of quasiparticles of different types and fluxes of their thermodynamic quantities. When the equilibrium is disturbed in one way or another, a similar role is played by functional expressions for the corresponding integral fluxes, the difference of which is equated to a fixed value, for example, the observed (density) flux for the difference in the integral fluxes of electrons $Q_e^+(x) - Q_e^-(x) = Q_*$.

The external physical environment, with its various flows falling on the surface of the structure, in one way or another, has different effects on the systems of quasiparticles. For example, the exchange of energy flows through the surface can be carried out even without the exchange of quasiparticles, through fluxes of different physical nature. Not in all cases, it is possible to correctly abstract from the influence of the external environment, at least in the near-surface region of the structure. Therefore, the equilibrium in this region always turns out to be conditional, depending not only on the properties of the surface of the solid-state layer, but also on the characteristics of various flows of the external environment in the circumstances under consideration.

Directly at the inner boundary between the layers in a solid structure, the integral fluxes of thermodynamic quantities in all systems of quasiparticles, in particular the energy fluxes $Q^{+}_{\varepsilon i}(x)$ and $Q^{-}_{\varepsilon i}(x)$, must be formed in accordance with the scheme shown in Figure 2a. In this case, one should take into account not only the properties of the boundary on its two sides, but also the difference in the quantum and kinetic properties of neighboring layers of solid materials, as well as the difference in thermodynamic characteristics in systems (flows) of quasiparticles. In addition, it should be understood that the losses in the integral fluxes $S^{+}_{a}Q^{+}_{i1}$ and $S^{-}_{a}Q^{-}_{i2}$ in one system of quasiparticles are redistributed over differential and, accordingly, integral fluxes of quasiparticles of other types according to the properties of the considered boundary (see Figure 2b in a multi-system version). Obviously, in a homogeneous thickness of a solid layer (far from its boundaries) with the scattering of differential fluxes on an elementary area located in a certain section of the layer, a similar physical picture takes place in equilibrium. Only in the latter case are the quantum and kinetic properties on the right and left sides of the cross-section the same, as are the scattering probabilities of differential fluxes and the distribution of thermodynamic quantities.

Here it is pertinent to recall about the structure, different in systems of quasiparticles, specific for each layer, the dependence of the categories “thin layer” and “homogeneous layer thickness” on external conditions in equilibrium and, with its various ways of violation. Moreover, any violation of equilibrium in the structure, corresponding to stationary external conditions, can also be characterized by the distribution of the considered thermodynamic quantities of integral fluxes of quasiparticles of different types. To do this, their definition should also be based on solutions “stitched” over the layers of the structure in all systems of quasiparticles under consideration, which should be self-consistent in all coefficients of the system of kinetic equations of the boundary value problem in each layer of the structure. The correct solution to such problems is impossible without the qualified implementation of a rather complex mathematical model on a computer.

The difference in the physical conditions of propagation and interaction of fluxes of charge carriers and other systems of quasiparticles in an inhomogeneous region (including at the boundary or the *p-n*-junction) and in a uniform layer thickness is, in particular, the appearance of an “ideality factor” in the dependence of the current-voltage characteristics of the structure with a potential barrier. In the characteristic, it is a factor for the “usual” temperature of the *p-n*-structure. It is clear that this factor, an empirically determined coefficient, is a certain simplification of the description of the real physical picture that occurs in quasiparticle systems mainly in the *p-n*-junction region. This factor largely determines the slope of the volt-ampere (I-U) characteristic.

In a *p-n*-junction structure used as the base of a solar cell, the ideality factor largely determines the efficiency of photoelectric conversion, since it strongly affects the “fill factor” FF (fill factor) I-U-characteristics “in the light”. When a solar cell is illuminated with concentrated solar radiation, the role of the interaction of fluxes of quasiparticles of different kinds turns out to be even more significant. In the rational development and creation of a high-power solid-state laser, it is also necessary to take into account the influence of fluxes of quasiparticles of different kinds on their propagation. The role of the interaction of different systems of quasiparticles of a solid structure with an N-or S-shaped current-voltage characteristic can also be significant.

The general physical picture of the propagation of fluxes of quasiparticles of different types over the thickness of a plane-parallel solid-state structure is outlined here in sufficient detail. Nevertheless, a detailed discussion of the complete mathematical model of the influence of differential fluxes of quasiparticles of different types on the propagation of each other near the boundary and in a homogeneous or inhomogeneous thickness of a separate layer and a layer in a solid structure, especially a thin one, requires special consideration. This requires fundamental research, a series of various technological, physical and computer experiments, as well as the scientific validity of confidence in the adequacy of the interpretation of various experimental data.

Only after that, with the accumulated baggage of new specialized knowledge in the field of kinetic theory and thermodynamics of an inhomogeneous solid-state medium, it is “economically” reasonable to start developing optimal multilayer structures of solid-state structures for various purposes, including cascade solar cells. In this case, the costly search for the optimal design of a structure for a specific purpose, consisting of a variety of solid materials, and, accordingly, technological modes and methods of its growth will be rationally purposeful and economically minimized in terms of various costs associated with research in general.

Considering the important scientific and great-applied technical significance, as well as the significant volume of these studies, it seems that at the initial stage it is rational to carry out them jointly by scientists from different countries: theorists, experimenters and technologists working in the field of solid-state physics, as well as highly qualified programmers and engineers.

7. Conclusions

Within the framework of the kinetic theory in the relaxation time approximation, the physical picture of the propagation of differential and integral fluxes of charge carriers near the boundary of an isotropic layer of a plane-parallel solid-state structure both in equilibrium and in its violation is considered. In this case, the possible exchange of quasiparticles of different types between the layers of the solid structure was taken into account. The reasons influencing the propagation of differential flow in this area are indicated. These include not only the appearance of an electric field $E(x)$ at the boundary in equilibrium and its modification when the equilibrium is disturbed, but also a change in the coordinate and angular dependence of the relaxation length of fluxes $l_e(x, k, \Omega)$ in the same region, as well as some modification distribution of other characteristic thermodynamic quantities.

The necessity of a self-consistent solution of the system of kinetic equations and determination of its coefficients, in particular $E(x)$ and $l_e(x, k, \Omega)$ for electrons, as well as the distributions of thermodynamic quantities, is substantiated in order to obtain greater reliability of the mathematical model of propagation of quasiparticle fluxes near the boundary and through it. The need for self-consistency of the solution of the kinetic equation has not previously been reliably argued, and even more so it has not been used in kinetic theory before. The ideology of self-consistency in the theory of atoms was substantiated and successfully applied earlier when solving the Schrödinger equation by the Hartree-Fock method.

It is proposed to use the coordinate distribution of the flux density of thermodynamic quantities over the thickness of the structure in the systems of quasiparticles taken into account, which is mutually self-consistent with the propagation of the corresponding fluxes of quasiparticles. In this case, each system of quasiparticles can still be considered ideal, although the interaction of systems and their mutual influence on the propagation of flows are taken into account. This allows us to introduce a correct definition of the temperature and chemical potential of the integral flux of quasiparticles in each of the systems under consideration, which more adequately describes the physical picture of the propagation of fluxes in an inhomogeneous multilayer solid structure, especially in a thin layer.

The scientific and practical significance of the results obtained lies in the fact that the microscopic “kinetic” picture of the propagation of differential and integral fluxes of charge carriers and quasiparticles of other types in a solid-state structure is disclosed in detail. Adequate understanding of the features of the propagation of fluxes of quasiparticles of different physical nature through the boundary and near it, as well as in a uniform thickness of a solid layer, makes it possible to correctly take into account the distribution of macroscopic thermodynamic quantities in systems of quasiparticles over all layers of the structure with different quantum and kinetic characteristics.

A more reliable mathematical model of the propagation of quasiparticles, taking into account the interaction of their different systems, will make it possible to more reliably optimize the structure of multilayer solid-state structures of electronic devices, such as solar cells, LEDs, lasers, etc., in order to increase their efficiency and/or reduce their cost. The prospects of the obtained scientific results will be revealed even more after the development of the corresponding package of applied programs.

By correctly solving the system of kinetic equations in a solid layer with specified characteristics and matching the solution for all layers of the structure, it is possible to adequately determine not only the values of the coefficients (parameters) of each layer within the framework of the diffusion-drift theory, but also their various dependencies.

The main conclusion of this work is as follows. A solid-state structure is an inhomogeneous medium with a specific distribution of physical properties over its thickness, including all of its boundaries. In equilibrium and when it is violated, the propagation of differential and integral fluxes of quasiparticles of different kinds in an inhomogeneous medium has its own peculiarities, as does the associated distribution over the thickness of fluxes of thermodynamic quantities in the corresponding systems of quasiparticles, especially near the boundaries of the structure. Therefore, when developing modern multilayer solid-state structures, especially with thin layers, it is necessary to use the kinetic or quantum theory, which adequately takes into account physical processes and statistical phenomena that occur not only in homogeneous and inhomogeneous regions of the thickness of each layer, but also at all boundaries of the structure.

Adequate consideration of the features of the propagation of differential and integral fluxes of charge carriers and quasiparticles of other types, as well as fluxes of thermodynamic quantities associated with them, near and across the boundaries of the layers of a solid-state structure, including conventional ones, will make it possible to more purposefully select solid-state materials to create appropriate structures and carry out optimization of its design on the basis of a more complete and deeper mathematical model.

Conflict of interest

The author declares no competing financial interest.

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