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The Important Thermal and Kinetic Properties of Crystals and Their Calculations with the Use of the Gibbs Potentials

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In this work, the important thermal and kinetic characteristics of crystals are calculated. It was shown that in a state of thermodynamic equilibrium, the thermal properties of crystals are additive, and their value for an entire crystal is calculated by summing the values of thermal properties of the crystal lattice and the properties of the gas of free charge carriers in a crystal. These properties are fully characterized by the appropriate Gibbs potentials. In this work it was also shown that when the electric field $\vec{E}$ and temperature gradient $\nabla_{\vec{r}} T$ are created in a crystal, and this crystal is placed in the magnetic field with the magnetic inductance vector $\vec{B}$, then there the electric charge and heat transport processes begin to exist in the crystal. These processes are described by the generalized electric and heat conduction equations. The tensors and the scalar coefficients in these equations – these are the kinetic properties of the crystals. They describe the nature of their actual properties and they have widespread and pragmatic applications in modern solid-state electronics.

Keywords: Gibbs potential, chemical potential, entropy of a system, equations of neutrality.

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I. An elementary model of a crystal. The statistical sum of a crystal

Semiconductor crystals are composed of the structural particles – these are located within their volume. These particles create the crystal lattice that it has a symmetry. The particles are located in points which are called the lattice sites, and the space between them is called the interstitial site. Atoms, ions or molecules can become the structural particles of a crystal. There is quantum interaction between the particles and it holds them in the lattice sites.

In a crystal can exist the free charge carriers and these carriers are moving chaotically in the crystal interstitial site, when the crystal is in the thermodynamic equilibrium state. In semiconductor crystals, electrons with the charge e or positive holes with the charge $-e$ can be the free charge carriers. A collection of the charge carriers in the crystal is called the electron or hole gas, or called as the gas of the charge carriers. Within elementary classical theory, the gas of charge carriers in the thermodynamic equilibrium is treated as an ideal gas. Therefore, the laws for an ideal gas are also applied to the charge carrier's gas.

In the thermodynamic equilibrium state, there is not any action of forced fields on the crystal, and its temperature remains constant and the same value in all its points. It is agreed that in all crystal states its structural particles hamonically vibrate around their nodes, the directions of these vibrations are varying chaotically, and the charge carriers gas is moving chaotically in the interstitial sites of the crystal lattice. Furthermore, one is inclined to think that the system of structural particles and the system of charge carriers only weakly interact with each other. In this case, the grand statistical sum of the crystal Ξ_k is equal to the product of two statistical sums: the statistical sum of structure particles Ξ_N and the statistical sum of charge carriers gas Ξ_n. Thus, $\Xi_k = \Xi_N \Xi_n$.

Therefore, the crystal as a thermodynamic system, is composed of two thermodynamic subsystems of particles. One subsystem – this is the gas of charge carriers, this gas is considered to be an ideal. The other – this a set of structure particles, which harmonically and chaotically vibrate around nodes of crystal lattice.

Having this model of the crystal, we shall calculate its statistical sum Ξ_k which enables us to determinate all thermodynamic properties of the crystal.

In statistical theory of crystal properties [1-5] it was shown that thermal characteristics of large thermodynamic systems are described in terms of the logarithm of the grand statistical sum. But the logarithm $\ln\Xi_k = \ln\Xi_n + \ln\Xi_N$. Physically, it means that the thermal properties of the crystal are additive and they add the thermal characteristics of the crystal lattice to the thermal characteristics of the charge carriers gas.

Systems in a state of thermodynamic equilibrium are described by thermodynamic functions (or by thermodynamic potentials), which explicitly depend on some independent system's parameters. Thus, the thermodynamic functions, as mathematical functions, will characterise some material properties of the system in a state of thermodynamic equilibrium.

There are the following important thermodynamic functions:

1. The system internal energy U
2. The thermal function (or enthalpy) H
3. The free Helmholtz energy F
4. The thermodynamic potential (or free Gibbs energy) G
5. The Gibbs grand thermodynamic potential Ω
6. The entropy S
7. The specific heat capacity C_V

These functions are explicite functions of some system parameters, they fulfil some mathematical relationships and possess the following total differentials:

$$\begin{array}{llll}
1. & U=U(S,V,N), & U=F+TS, U=H-PV, & dU=TdS-PdV+mdN,\\
2. & H=H(S,P,N), & H=U+PV, & dH=TdS+VdP+mdN,\\
3. & F=F(T,V,N), & F=U-TS, & dF=-SdT-PdV+mdN,\\
4. & G=G(T,P,N), & G=F+PV=mN, & dG=-SdT+VdP+mdN,\\
5. & \Omega=\Omega(T,V,m), & \Omega=F-G=-PV, & d\Omega=-SdT-VdP-Ndm,\\
6. & S=S(U,V,N), & S=\left.(U-F)\middle/T\right., & dS=\dfrac{dU}{T}+\dfrac{P}{T}dV-\dfrac{m}{T}dN,\\
7. & C_V=\left(\dfrac{dU}{dT}\right)_V. & &
\end{array} \tag{1}$$

In the above formulas, V is the system volume, p is the pressure in the volume V, μ is the chemical potential of particles in the volume V.

These thermodynamic functions which describe material properties of a system in equilibrium state are calculated in statistical theory of thermal and kinetic properties of real systems. The real systems are composed of a very large amount of microparticles. For a limit of large numbers N, this collection of N microparticles satisfies the central limit theorem of large numbers. This theorem shows that the statistical laws of nature, which are based on mathematical probability theory, act in such systems.

The thermodynamic potentials (thermodynamic functions) are functions of the independent system's macroparameters, which fully describe its state. The functions belonging here are the system internal energy U, thermal function (or enthalpy) H, free Helmholtz energy F, thermodynamic potential (or free Gibbs energy) G, Gibbs grand thermodynamic potential Ω, entropy S, specific heat capacity C_V. With the use of the thermodynamic functions (potentials), all macrocharacteristics of the system can be calculated, and these potentials provide an explanation for a movement of physical and chemical processes in this system. Moreover, with the use of the thermodynamic functions (potentials) the conditions for equilibrium of thermodynamic systems can be established. There are conditions here, the maximum of a system entropy, minimum of a system free energy and minimum of the Gibbs potential. To describe systems with a variable amount of particles, the chemical potential μ has been introduced. This is a quantity which defines a change in energy of a system, when the number of its particles is increased by one.

The internal energy U – this is the energy of a thermodynamic system which is a function of its state. It includes all forms of all particles energies. In the state of equilibrium, the internal energy U is a total thermal energy of this system.

The enthalpy H – this is a function of its state which characterizes a change of the system thermal energy δQ for isobaric processes (processes occuring at constant pressure). Thus, under this condition $dH = \delta H$.

The free energy of the system F defines the value of a work δA for isothermic reversible processes that the system can do against to external forces. This work is equal to a change of the system free energy, that it is taken with the opposite sign, i. e., $\delta A = -dF$.

The thermodynamic Gibbs potential G – this is a function of the state of the thermodynamic system which characterizes reversible and irreversible isobaric-isothermal processes in the system. The thermodynamic Gibbs potential is constant during the reversible processes and it goes down during the irreversible processes.

The Gibbs grand thermodynamic potential Ω characterizes the pressure in the thermodynamic system of particles.

The entropy S – this is a function of the state, it gives the possibility to write up the second law of thermodynamics in a mathematical rigorous way.

The specific heat capacity C_V (per unit volume) is an important characteristics of the system, it is the amount of heat as it should be transferred to the system to raise its temperature by one degree kelvin. Therefore, the heat capacity at constant volume of the crystal is given as:

$$C_V = \frac{dU}{dT}.$$

In statistical physics it was shown [1-5] that all thermodynamic systems characterized by given above thermodynamic functions are descibed by the Gibbs grand canonical distributions $\Omega = -kT\ln(\Xi)$. Thus, these thermodynamic functions are expressed in terms of the Gibbs grand canonical potential, and they are given here by the following algorithmic formulas:

$$U = \Omega - \left(\frac{d\Omega}{dm}\right)_T m - \left(\frac{d\Omega}{dT}\right)_m T, \tag{2}$$

$$H = -\left(\frac{d\Omega}{dm}\right)_T m - \left(\frac{d\Omega}{dT}\right)_m T, \tag{3}$$

$$F = \Omega - \left(\frac{d\Omega}{dm}\right)_T m, \tag{4}$$

$$G = -\left(\frac{d\Omega}{dm}\right)_T m, \tag{5}$$

$$\Omega = -kT\ln\Xi, \tag{6}$$

$$S = -\left(\frac{d\Omega}{dT}\right)_m = \frac{U-F}{T}, \tag{7}$$

$$C_V = \left(\frac{dU}{dT}\right)_V, \tag{8}$$

$$PV = -\Omega = kT\ln(\Xi), \tag{9}$$

$$N = -\left(\frac{d\Omega}{dm}\right)_T. \tag{10}$$

Equation (9) is called the thermodynamic equation of a state of the many-particles system, this system has the volume V and the particles create the pressure V in its volume.

Hence, it follow that the problem of calculation of the thermodynamic functions of the system – this is the problem of calculation of its grand statistical sum Ξ.

As it was shown in the works [1-2] and in works [3-5], the thermal properties of the crystal lattice and the current carriers gas in the crystal are fully described by the following Gibbs grand potentials, respectively:

$$\begin{aligned}\Omega_D &= -kT\ln\left(\Xi_N\right) = 9NkT\left(\frac{T}{q}\right)^3 \int_0^{\frac{q}{T}} x^2\ln\left(1-\exp(-x)\right)dx = \\ &= 3NkT\left[3\ln\left(1-\exp\left(-\frac{q}{T}\right)\right) - D\left(\frac{q}{T}\right)\right],\end{aligned} \tag{11}$$

$$\begin{aligned}\Omega &= -kT\ln\left(\Xi_n\right) = -V\int_0^{\infty}\frac{G(e)}{\left(\exp\left(\frac{e-m}{kT}\right)+1\right)}de = \\ &= -V\int_0^{\infty} G(e)\,f_0(e)\,de.\end{aligned} \tag{12}$$

Formula (11) is called the Debye's interpolation formula. In this formula, the following notations are used: $\theta = \frac{\hbar\omega_{max}}{k}$ is the Debye temperature which depends on the nature of the crystal, $D(Z) = \frac{3}{Z^3}\int_0^Z \frac{x^3}{(\exp(x)-1)}dx$ is the Debye function, N is the number of the crystal structure particles.

In formula (12), $f_0(\varepsilon)$ is the well-known Fermi-Dirac distribution function, $G(\varepsilon) = \int_0^\varepsilon g(\varepsilon)d\varepsilon$, $g(\varepsilon)$ is the density of states lying in allowed band, ε is the quantum particle energy which depends on its quasimomentum vector $\vec{p}$. The function $\varepsilon(\vec{p})$ is named the dispersion relation. According to the quantum theory laws, the exact dispersion relation is a periodic and even function of the vector $\vec{p}$. Formulas (11) and (12) are detailed described in the cited works.

Having the thermodynamic potential Ω_D, the known algorithmic formulas of kinetic theory of crystals properties permit the calculation of all thermodynamic properties of the crystal lattice, under the condition that the chemical potential of phonons is equal to zero ($\mu = 0$). Thus, we have:

$$U_D = \Omega_D - \left(\frac{d\Omega_D}{dT}\right)T = 3NkTD\left(\frac{q}{T}\right), \tag{13}$$

$$\begin{aligned}H_D &= -\left(\frac{d\Omega_D}{dT}\right)T = \\ &= U_D - F_D = NkT\left[4D\left(\frac{q}{T}\right) - 9\ln\left(1-\exp\left(-\frac{q}{T}\right)\right)\right],\end{aligned} \tag{14}$$

$$F_D = \Omega_D = 3NkT\left[3\ln\left(1-\exp\left(-\frac{q}{T}\right)\right) - D\left(\frac{q}{T}\right)\right], \tag{15}$$

$$G_D = 0, \tag{16}$$

$$\Omega_D = F_D = 3NkT\left[3\ln\left(1-\exp\left(-\frac{q}{T}\right)\right) - D\left(\frac{q}{T}\right)\right], \tag{17}$$

$$\begin{aligned}S_D &= -\left(\frac{d\Omega_D}{dT}\right) = \frac{U_D - F_D}{T} = \\ &= Nk\left[4D\left(\frac{q}{T}\right) - 9\ln\left(1-\exp\left(-\frac{q}{T}\right)\right)\right],\end{aligned} \tag{18}$$

$$C_{VD} = 3Nk\left[4D\left(\frac{q}{T}\right) - \frac{3}{\left(\exp\left(\frac{q}{T}\right)-1\right)}\right], \tag{19}$$

$$(PV)_D = -\Omega_D = 3NkT\left[D\left(\frac{q}{T}\right) - 3\ln\left(1-\exp\left(-\frac{q}{T}\right)\right)\right]. \tag{20}$$

The general thermal properties of the crystal are additively added the thermal properties of the crystal lattice and thermal properties of the free charge carriers gas. The free charge carriers' gas – this is the Fermi gas. Its thermal properties are fully described by the Gibbs potential Ω (12) and they have the forms:

$$U = \Omega - \left(\frac{d\Omega}{dm}\right)_T m - \left(\frac{d\Omega}{dT}\right)_m T = N_e \langle e g(e) \rangle, \qquad (21)$$

$$H = -\left(\frac{d\Omega}{dm}\right)_T m - \left(\frac{d\Omega}{dT}\right)_m T = N_e \left\langle \frac{d}{de}\big(eG(e)\big) \right\rangle, \qquad (22)$$

$$F = \Omega - \left(\frac{d\Omega}{dm}\right)_T m = N_e \big(m - \langle G(e) \rangle\big), \qquad (23)$$

$$G = -\left(\frac{d\Omega}{dm}\right)_T m = N_e m, \qquad (24)$$

$$\Omega = -kT \ln(\Xi_n) = -V \int_0^\infty G(e) f_0(e) de, \qquad (25)$$

$$S = -\left(\frac{d\Omega}{dT}\right)_m = \frac{U - F}{T} = N_e k \left(\left\langle \frac{d}{de}\big(eG(e)\big) \right\rangle - m \right) \qquad (26)$$

$$C_V = \left(\frac{dU}{dT}\right)_V, \qquad (27)$$

$$PV = -\Omega = kT \ln(\Xi_n) = N_e \langle G(e) \rangle, \qquad (28)$$

$$N = -\left(\frac{d\Omega}{dm}\right)_T. \qquad (29)$$

In the above formulas, the average operator is denoted by the angle brackets $<\ldots>$:

$$< \varphi > = \frac{J(\varphi(\varepsilon))}{J(g(\varepsilon))} = \frac{\int_0^\infty \varphi(\varepsilon) f_0(\varepsilon) d\varepsilon}{\int_0^\infty g(\varepsilon) f_0(\varepsilon) d\varepsilon}.$$

II. Elements of statistical theory of non-equilibrium thermodynamics. Kinetic properties of crystals

In the preceding section, the thermodynamic properties of systems in a state of thermodynamic equilibrium were discussed. The necessary equilibrium conditions for this state are that the temperature and chemical potential should be constant throughout all points in the system. If one of these conditions does not hold, then there are nonequilibrium processes in this system. These processes bring the system into thermodynamic equilibrium state. A crystal in equilibrium state (as a thermodynamic system) can be removed from equilibrium by the action of the electric field$\vec{E}$, chemical potential gradient $\nabla_{\vec{r}}\mu$, or temperature gradient $\nabla_{\vec{r}}T$ in the crystal. These fields may exist simultaneously in the crystal. In the presence of these there are the fluxes of mass, energy and charge. They are described by the first and second laws of nonequilibrium thermodynamics:

$$\frac{dU_e}{dt} = -div\vec{q} + \vec{j}\vec{E}$$

$I \ - (the\ first\ law\ of\ nonequilibrium\ thermodynamics)$;

$$\frac{dS_e}{dt} = \frac{1}{T}\left(\vec{j}\vec{E} - \frac{\vec{q}\nabla_{\vec{r}}T}{T}\right),$$

$II \ - (the\ second\ law\ of\ nonequilibrium\ thermodynamics)$.

In the above laws, $\vec{j}, \vec{q}$ are the vectors of the electric current density and heat flow, and U_e, S_e are respectively the internal energy and entropy of the system.

In statistical physics it was shown that, when there is an increase of the entropy in the thermodynamic system, the processes of heat and electric charge transport (processes of heat and electric conduction) occur. Conversely, when the processes of heat and electric charge transport occur in the system, its entropy inreases. Thus, we have:

$$\frac{dS_e}{dt} = \frac{1}{T}\left(\vec{j}\vec{E} - \frac{\vec{q}\nabla_{\vec{r}}T}{T}\right) \geq 0.$$

In nonequilibrium thermodynamics, it was shown that when the electric field $\vec{E}$ and temperature gradient $\nabla_{\vec{r}}T$ are created in conducting medium, and next place this crystal in the magnetic field with the magnetic inductance vector $\vec{B}$, then there the electric charge and heat transport processes begin to exist in the crystal. These processes are described by the following generalized electric and heat conduction equations:

$$\vec{j} = \big(\sigma_{ik}(\vec{B})\big)\vec{E} - \big(\beta_{ik}(\vec{B})\big)\nabla_{\vec{r}}T, \qquad (30)$$

$$\vec{q} = \big(\gamma_{ik}(\vec{B})\big)\vec{E} - \big(h_{ik}(\vec{B})\big)\nabla_{\vec{r}}T, \qquad (31)$$

Equations (30) and (31) describe the response of conducting medium to the action of the electric field, temperature gradient and magnetic field. The phenomenological constants in equations (30), (31) $(\sigma_{ik}(\vec{B})), (\beta_{ik}(\vec{B})), (\gamma_{ik}(\vec{B})), (h_{ik}(\vec{B}))$ – these are the tensors of kinetic coefficients. These tensors describe numerous matter properties of the conducting medium (i. e., this crystal). They have the well-known properties of the Onsager symmetry.

The kinetical properties of the conducting crystals are determined by the concentration of the free charge carriers in the crystals and by the character of their motion throughout the crystal interstitial site.

In equilibrium state, the free charge carriers are moving chaotically, their average energy is conserved, and the entropy of the system of these carriers obtains its maximum value. This is an equilibrium gas of the charge carriers.

The presence some drift perturbations in the crystal, that is, the electric field $\vec{E}$, the temperature gradient $\nabla_{\vec{r}}T$ (these perturbations may exist simultaneously in the crystal), will remove the charge carriers' gas out from equilibrium and turn it into the non-equilibrium particles' ensemble. In this case, the drift force $\vec{F}_d$ will be act on every particle of charge ze, according to [1 - 5]:

$$\vec{F}_d = ze\vec{E}_d; \quad \vec{E}_d = \vec{E} - \left(\frac{k}{ze}\right)\left(\frac{e - m}{kT}\right)\nabla_{\vec{r}}T, \qquad (32)$$

where e is the electron charge, $z = \pm 1$ is the charge sign, ε is the average energy of the charge carrier, μ is the chemical potential of the charge carriers, k is the Boltzmann's constant, T is the crystal temperature.

As a result of the action of the drift force $\vec{F}_d$, all current carriers start to move in a rectilinear way, and they will have the drift velocity $\vec{v}_d$. This velocity depends on the force $\vec{F}_d$ as well as the crystal's properties.

The presence of the drift velocity $\vec{v}_d$ creates a particle flow. As it takes place, there is the electric charge and heat (energy) transport. Therefore, the collection of charge carriers in crystals, when there are drift fields, turns into the grand canonical nonequilibrium ensemble with the varying amount of particles.

As it was shown in the work [1], taking into consideration a spin degeneracy, this grand canonical ensemble is characterized by the following Gibbs grand canonical potential:

$$\Omega = -2kT\sum_{\vec p}\ln\left\{1+\exp\left(\frac{\mu+\Delta\mu_{\vec p}-\varepsilon_{\vec p}}{kT}\right)\right\}, \qquad (33)$$

In the above formula, $\vec{p}$ is the wavevector of the charge carrier, $\varepsilon_{\vec{p}}$ is the energy dispersion relation of the charge carriers, and $\Delta\mu_{\vec{p}}$ is the change in the one particle chemical potential (free energy per particle) by the action of these perturbations (these will remove the crystal out from the equilibrium state). When these perturbations are absent, $\Delta\mu_{\vec{p}} = 0$.

The values $\Delta\mu_{\vec{p}}$ were calculated in the work [4], where it was shown that $\Delta\mu_{\vec{p}}$ is an odd function of the vector $\vec{p}$, and it depends on the vector of electric field $\vec{E}$, temperature gradient $\nabla_{\vec{r}}T$ and vector of magnetic inductance $\vec{B}$, when the crystal is under these perturbations.

As it was shown in the cited works, the use of the thermodynamic potential (33) leads to the following generalized equations of the electric and heat conductions:

$$\begin{aligned}\vec E &= \left(\rho_{ij}(\vec B)\right)\vec j + R(\vec B)\cdot\left[\vec B\times\vec j\right]+\\ &+\left(\alpha_{ij}(\vec B)\right)\nabla_{\vec r}T + N(\vec B)\left[\vec B\times\nabla_{\vec r}T\right]\end{aligned}, \qquad (34)$$

$$\begin{aligned}\vec q &= \left(\pi_{ij}(\vec B)\right)\vec j + P(\vec B)\cdot\left[\vec B\times\vec j\right]-\\ &-\left(\chi_{ij}(\vec B)\right)\nabla_{\vec r}T + S(\vec B)\left[\vec B\times\nabla_{\vec r}T\right]\end{aligned}, \qquad (35)$$

In the above equations, the symmetric tensors $\left(\rho_{ij}(\vec{B})\right)$, $\left(\alpha_{ij}(\vec{B})\right)$, $\left(\pi_{ij}(\vec{B})\right)$, $\left(\chi_{ij}(\vec{B})\right)$ – these are respectively, the material tensors of the resistivity, Seebeck effect, Peltier effect and thermal conductivity of the crystal. These tensors should be experimentally determined or theoretically calculated. They are even function of the magnetic inductance vector $\vec{B}$.

The coefficients $R(\vec{B})$ and $P(\vec{B})$ – these are the coefficients of transverse galvanomagnetic Hall and Ettingshausen effects, and the coefficients $N(\vec{B})$ and $S(\vec{B})$ are the coefficient of transverse thermomagnetic Nernst-Ettigshausen and Righi-Leduc effects. They are even function of the magnetic inductance vector $\vec{B}$, that is: $R(\vec{B}) = R(-\vec{B})$, $P(\vec{B}) = P(-\vec{B})$, $N(\vec{B}) = N(-\vec{B})$, $S(\vec{B}) = S(-\vec{B})$.

All these just given tensors and coefficients are called the kinetic properties of the crystals.

In equations (34), (35), the vector product are denoted by the square brackets.

The analysis of equations (34), (35) shows that in the presence of a magnetic field, an isotropic crystal becomes anisotropic, and the relativity simple processes of the electric and heat conduction will become more complicated. In this case, the additional transverse galvanomagnetic and thermomagnetic effects there occur.

The galvanomagnetic effects are produced by the action of a magnetic field on the omic part of the electrical current, and the thermomagnetic effect – by the action of this field on the thermal part of the current, accordingly to the generalized equations of the electric conduction (34).

The kinetic tensors and coefficients in equations (34), (35) describe the nature of the important kinetic properties of conducting medium, they are of pragmatic significance for modern solid-state electronics, where crystal of different nature are used in the manufacturing.

In the cited works [1-5], it was shown that all kinetic properties of crystals are calculated with the use the following main algorithmic functional:

$$J(i,j,B_3,\mu^{\bullet},T) = \int_0^{\infty}\left(\frac{\varepsilon}{kT}\right)^i\frac{u(\varepsilon)^j}{d(B_3)}G(\varepsilon)\left(-\frac{df_0}{d\varepsilon}\right)d\varepsilon\,,$$

$$d(B_3) = 1+\left(u(\varepsilon)B_3\right)^2. \qquad (36)$$

In the above formula, $G(\varepsilon) = \int_0^{\varepsilon} g(\varepsilon)d\varepsilon$, $g(\varepsilon)$ is the density of the energy states of charge carriers lying in allowed energy bands, $f_0(\varepsilon) = \left(\exp(\frac{\varepsilon-\mu^{\bullet}}{kT}) + 1\right)^{-1}$, $u(\varepsilon)$ is the scattering function which describes the effect of scattering processes of the current carriers by the crystals' defects on the crystal kinetic properties (this scattering function is a non-averaged charge carrier mobility), B_3 is the component of the magnetic inductance vector $\vec{B}$ in the crystal , which is normal to vectors $\vec{E}$, $\nabla_{\vec{r}}T$.

It is clear from the analysis of the main algorithmic functional (36) that the kinetic properties of the crystal depend on the energy dispersion relation of the charge carriers, the scattering function and the chemical potential $\mu^{\bullet} = \frac{\mu^{\bullet}}{kT}$.

This analysis of the computational algorithms of thermal properties of a crystal shows that all these properties analytically depend on the energy dispersion relation of the charge carriers and the chemical potential $\mu^{\bullet}$.

The problems of calculations of such quantities, that the crystals' thermal and kinetic properties analytically depend on them, are described in the work [4]. In this work, the methods of calculations of the thermal and kinetic properties for $2D$ and $1D$ crystals are given.

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Важливі теплові і кінетичні властивості кристалів та їх розрахунки за допомогою потенціалів Гіббса

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В даній роботі розраховані важливі теплові і кінетичні характеристики кристалів. Показано, що в стані термодинамічної рівноваги теплові властивості кристалів аддитивно складаються із теплових властивостей кристалічної гратки і газу вільних носіїв зарядів в кристалі. Ці теплоти повністю описуються відповідними потенціалами Гіббса.У роботі також показано, що коли в провідному кристалі створити електричне поле з напруженістю $\vec{E}$, та градієнт температури $\nabla_{\vec{r}} T$ і помістити цей кристал в магнітне поле з вектором індукції $\vec{B}$, то в ньому виникають процеси перенесення електрики і теплоти, які описуються відомими узагальненими рівняннями електропровідності і теплопровідності. Тензори і скалярні коефіцієнти, які входять в склад цих рівнянь, це–кінетичні властивості кристалів. Вони описують природу їх актуальних властивостей і мають широке прагматичне застосування в сучасній твердотілій електроніці.

Ключові слова: потенціал Гіббса, хімічний потенціал, ентропія системи, рівняння нейтральності.