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Physics

Melting Electronic Mechanism in Covalent Crystal Substances and Nanostructures, Calculation of Heat Capacity according to Interatomic Chemical Bonding

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(Presented by Academy Member G.Chagelishvili)

ABSTRACT. Values of bonding energies of sp^3 and sp^2s^- hybrid bonding are calculated in the paper. These calculations are performed according to the conception of the influence of anti-bonding quasi-particles on the interatomic bonding force when the bonding particle takes an anti-bonding position. Melting process of covalent crystals is considered and the critical concentration of anti-bonding quasi-particles, at which the melting process begins, is defined. And it may be caused by action of light, injection of charge carriers and other ways. The heat capacity of Einstein's model of solid state in 3D crystal is calculated as well as in 2D systems.
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***Key words:** melting, heat capacity.*

1. Introduction. The theory of specific heat of solid state, as is known, was created by Einstein [1, 2] and then by Debye. Einstein's theory is based on Einstein's model of solid state. According to this model, all the atoms of the solid state have the same oscillation frequency, but in Debye's model atoms' oscillation is presented as a spectrum of the frequency of isotropic continuum's flexible oscillations. So, in the low temperature range the results of Einstein's and Debye's theories do not differ very much from each other, though in some cases Debye's theory is very close to experimental results. In high temperature ranges, the results of Einstein's and Debye's theories are similar, and both turn to Deulong's and Petit's rules. According to many experimental data [1, 3-5], we can agree to the very important results that in low temperature, as well as in high temperature ranges, Deulong's and Petit's rules for the general, three-dimensional crystal states (3D systems) do not work. Neither do Einstein's and Debye's theories in 2D quantized systems [4, 6-8]. Heat capacity of any substance depends on the frequency of atoms' oscillation. This frequency depends on the interatomic bonding energy. In 1984 a group of some authors offered a conception, which says that interatomic bonding energy depends on the correlation of bonding and anti-bonding quasi-particles (quasi-free electrons and holes in semiconductors). Actually, this idea is the result of simplest hydrogen molecule analogy: bonding energy in hydrogen molecule is maximal, when it's performed by two, different in spin, electrons. These electrons are called bonding electrons. They are located in the singlet level (bonding level) of molecule. If we transfer one of them to the triplet level (anti-bonding level), then the molecule will collapse. Or if we add to this molecule third electron, (it will take the anti-bonding level, because bonding level is full) bonding energy will decrease. If we view solid as one huge molecule, then, according to type of interatomic bonding and correlation of bonding and anti-bonding quasi-particles we can speak about bonding force. According to the given

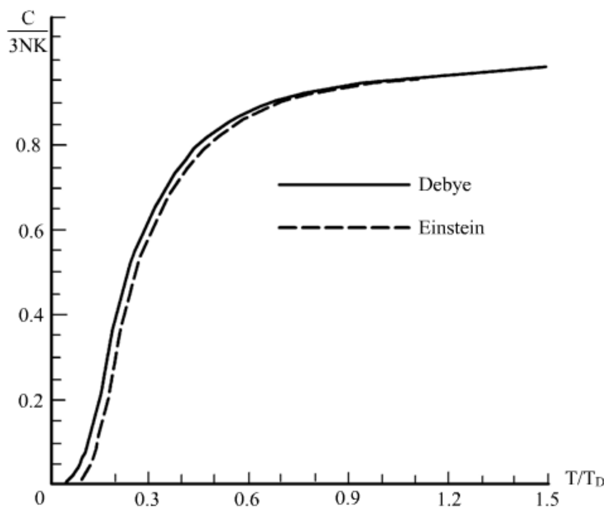

Fig. 1. Dependence between heat capacity and temperature of crystal lattice according to Debye's and Einstein's theories (T_D is Debye's Temperature).

conception melting, diffusion, defects precipitation, photomechanical and photo-stimulated diffusion occurrences in covalent crystals were investigated successfully in [9-12]. Let us calculate the heat capacity for covalent crystals.

2. Conception of collective bonding force decreasing in covalent crystals and its clarity. In covalent crystals chemical bonding between neighbor atoms is realized with sp^3 hybrid bonding. Separately, in one atom of covalent substance there are four electrons on the last orbit: two of them are *s* electrons and the other two – *p* electrons. There is ΔE_{sp} energetic difference between these *s* and *p* atoms. There are 2 vacancies in *s* state and 6 in *p* state (Fig. 2a). If the molecule is made of atoms like this, there appears virtual sp^3 hybrid level, where we have 8 places and all 4 (2 *s* and 2 *p*) electrons are virtually situated in them (Fig. 2b). After electrical and magnetic influence, sp^3 hybrid level collapses into

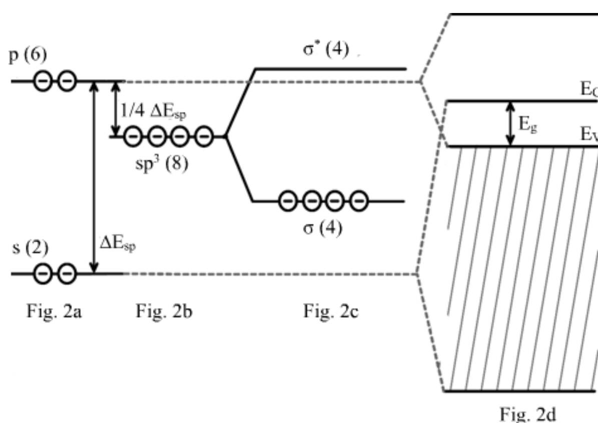

Fig. 2. Scheme of converting molecular orbital to zone pattern

bonding σ and anti-bonding σ^* levels. At each of them we have 4 places. All four electrons of the given atom occupy σ bonding level and σ^* anti-bonding level is empty (Fig. 2c). These full σ levels in the whole substance create a valence band which is full with bonding electrons and σ^* levels create an empty conducting band. One part of the collapsed *s* state of atom is the bottom of the conducting band and the other – bottom of the valence band, while one part of the collapsed *p* state is the top of the conducting band and the other part – top of the valence band (Fig. 2d). These results are known from [13].

When one σ electron moves to the anti-bonding level, there appears another anti-bonding particle: anti-bonding hole. As the top of the valence band is one part of *p* state, the wave function of the electron in this part has *p* symmetry and at the bottom of the conducting band the function has *s* symmetry. So, electron's movement from bonding level to anti-bonding level causes not only a decrease of the interatomic bonding force, but change of bonding symmetry. This means increasing part of symmetry in linked electrons' wave function (we will consider this question in detail in the next section). According to the conception which was offered by authors of [14], decrease of bonding force and change of bonding symmetry take place between these atoms, where the anti-bonding quasi-particles "travel". Based on this conception, melting of the substance will begin when the concentration of anti-bonding quasi-particles is so great that during one cycle of atom, anti-bonding quasi-particles will "travel" in all the atoms of the substance. We think that this conception is valid, but it needs freeing from some inconsistency which is caused by the conditions listed below: at a given temperature the quasi-impulse of anti-bonding quasi-particles is $P \sim \sqrt{3m^*KT}$. m* is effective mass of the quasi-particle. Based on the given conception $d \sim \frac{1}{\sqrt[3]{N}}$. According to the Heisenberg principle, $Pd \geq 2\pi\hbar$ which means that $\frac{\sqrt{3m^*KT}}{2\pi\hbar\sqrt[3]{N}} \geq 1$ condition must be met, but even for the highest melting temperature $T = T_m$, e.g. for silicon $\frac{\sqrt{3m^*KT}}{2\pi\hbar\sqrt[3]{N}} \leq 0{,}1$ so, the Heisenberg principle isn't met. This means that it is unable to use even the classical rules of statistics. As we remain in the frame of conception of collective decreasing of bonding force by anti-bonding quasi-

particles [14], our method is based on the wave nature of quasi-particles. In semiconductors quasi-free particles' (electrons and holes) wave function in effective mass approximation may be expressed by de Broglie's wave instead of Bloch's function. In terms of this, one quasi-particle decreases the bonding force and changes the symmetry not only of one atom but a whole group of atoms that are placed in a definite part of de Broglie's wave length. de Broglie's wave length for quasi-free electrons and holes is: $\lambda_{De} = \frac{2\pi\hbar}{\sqrt{3m_e KT}}$; and $\lambda_{Dp} = \frac{2\pi\hbar}{\sqrt{3m_p KT}}$. m_e is effective mass of quasi-free electron and m_p – effective mass of quasi-free hole. The capacities of spheres with diameters λ_{De} and λ_{Dp} are: $V_{De} = \frac{\pi}{6}\lambda_{De}^3$; $V_{Dp} = \frac{\pi}{6}\lambda_{De}^3$. As we are focused on semiconductors, so $n=p=n_i$. $2n_iV$ is the number of all anti-bonding quasi-particles in the entire V capacity, and $n_iV\left(V_{De}+V_{Dp}\right) = \frac{\pi}{6}n_i\left(\lambda_{De}^3+\lambda_{Dp}^3\right)V$ is the sum of capacities of all the spheres with diameters λ_{De} and λ_{Dp}. At melting temperature $q_D(T_m) = \frac{\pi}{6}n_i(T_m)\left(\lambda_{De}^3(T_m)+\lambda_{Dp}^3(T_m)\right) > 1$. e.g. in silicon $q_D(T_m)$=3.7, in germanium $q_D(T_m)$=6.5 and in GaAs $q_D(T_m)$=6.4. It's definite that $n_iV\left(V_{De}+V_{Dp}\right) > V$. If we consider that anti-bonding quasi-particles decrease interatomic bonding force and change symmetry of wave function in atoms which are located on $\lambda_e = \frac{\lambda_{De}}{\sqrt[3]{q_0(T_m)}}$, $\lambda_p = \frac{\lambda_{De}}{\sqrt[3]{q_0(T_m)}}$ length, then the value $q = \frac{\pi}{6}n_i\left(\lambda_e^3+\lambda_p^3\right)$ will change at the melting temperature like this:

$$q(T_m) = \frac{\pi}{6}n_i(T_m)\left(\lambda_e^3(T_m)+\lambda_p^3(T_m)\right) = 1. \qquad (1)$$

We think that this is the melting condition. It means that the influence of anti-bonding quasi-particles spreads everywhere in the entire crystal. When anti-bonding quasi-particles are not created by thermal energy but in a different way, e.g. by light or pressure etc, then $T\neq T_m$, which means that conditions of changing bonding force and symmetry of wave function look like this:

$$\frac{\pi}{6}n_k\left(\lambda_e^3(T)+\lambda_p^3(T)\right) = 1 \qquad (2)$$

So if melting is caused by heat transfer, then critical concentration of anti-bonding quasi-particles is the number of these particles at the melting temperature in a given crystal. If melting is caused by light (laser), etc. then the concentration of quasi-particles must be given with (9) condition:

$$n_k = \frac{3(3KT)^{3/2}q(T_m)}{4\pi^2\hbar^3}\left(\frac{m_e^{3/2}m_p^{3/2}}{m_e^{3/2}+m_p^{3/2}}\right) \qquad (3)$$

3. Change of wave function symmetry and decrease of bonding force by anti-bonding quasi-particles in covalent crystals. As we said above, the bonding between atoms in covalent crystals is effected with sp^3 hybrid wave function. First, let's calculate the energy of covalent bonding in an ideal covalent crystal. When it isn't excited, calculation can be made using the LCAO method. We choose only one direction, because all the other directions are the same. The function of this sp^3 hybrid bonding in direction, which is given in Fig. 3, looks like this [15]:

$$\Phi_{1,2}(r) = \frac{1}{2}\Psi_s(r)+\frac{\sqrt{3}}{2}\Psi_{px}(r). \qquad (4)$$

Covalent bonding energy between 1 and 2 atoms is [16]:

$$V_c^{(0)} = <\Phi_1(1)|\mathrm{H}|\Phi_1(2)> = -\frac{1}{4}\left(V_{ss\sigma}-2\sqrt{3}V_{sp\sigma}-3V_{pp\sigma}\right), \qquad (5)$$

where

$$V_{ss\sigma} = <\psi_s(1)|\mathrm{H}|\psi_s(2)>;$$

$$V_{sp\sigma} = <\psi_s(1)|\mathrm{H}|\psi_{px}(2)> = -<\psi_{px}(1)|\mathrm{H}|\psi_s(2)>;$$

$$V_{pp\sigma} = <\psi_{px}(1)|\mathrm{H}|\psi_{px}(2)>.$$

These matrix elements are given in [11].

Now let us consider the case when an electron tears off the sp^3 hybrid bonding, moves to interatomic space

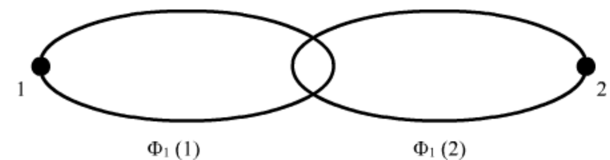

Fig. 3. One of the sp^3 bonding orbital shapes

(in conducting band), and a hole appears in its place. Symbolically, we can call this transition $sp^3 \rightarrow sp^2s^-$, which means that one of the 4 bonding electrons moved to anti-bonding orbital, which has *s* symmetry. If we choose the general sp^3 hybrid bonding (4) function as the basic function (as it was in the previous case), we will provide the principle of bonding maximality and the fact that in this state, from where the bonding electron comes, the probability of catching another electron, rises twice. Using the LCAO method, sp^2s^- bonding wave function is given as:

$$\Phi_1^{(1)}(r) = \frac{1}{2\sqrt{5}}\left\{\left(\sqrt{2}+3\right)\Psi_s(r) + \sqrt{3}\left(\sqrt{2}-1\right)\Psi_{px}(r)\right\}. \quad (6)$$

s and *p* function coefficients can be considered as "parts of state", when sp^3 hybrid bonding is changed with sp^2s^- one. Generally, in sp^3 hybrid bonding part of *p* state is 3 times greater than part of *s* state, but in the case of sp^2s^- bonding, part of *s* state is $\left(\frac{\sqrt{2}+3}{\sqrt{3}\left(\sqrt{2}-1\right)}\right)^2 \sim 40$ times greater, than the part of *p* state. So this is isotropization of bonding.

In regard to covalent bonding energy, for the given state it looks like this:

$$V_c^{(1)} = \langle \Phi_1^{(1)}(1)|H|\Phi_1^{(1)}(2)\rangle = \frac{1}{20}\left\{\left(11+6\sqrt{2}\right)V_{ss\sigma} - \right.$$

$$\left. -2\sqrt{3}\left(2\sqrt{2}-1\right)V_{sp\sigma} + 3\left(3-2\sqrt{2}\right)V_{pp\sigma}\right\} \quad (7)$$

4. Heat capacity calculation. We will calculate the heat capacity for covalent crystals in Einstein's solid state model according to the given results. In this model, in a substance which is built with *N* number of atoms, the oscillation energy is:

$$\overline{E} = \frac{3N\hbar\omega}{e^{\frac{\hbar\omega}{KT}} - 1}. \quad (8)$$

In this equation zero-point oscillation energy is ignored, because only these oscillations take part in the interaction with electrons that are caused by energy higher than zero point energy. Generally, atoms' oscillation frequency depends on covalent bonding energy between them [16, 17]:

$$\omega = 8\sqrt{\frac{V_c}{3d^2M}\left(1+\frac{V_0}{V_C}\right)^{-3/2}}, \quad (9)$$

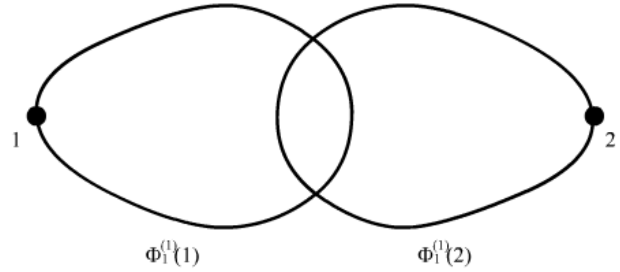

Fig. 4. Shape of sp^2s^- orbital in one of the directions

where $V_0 = \frac{\varepsilon_s^{(1)} - \varepsilon_s^{(2)}}{2}$ is ionic bonding energy on hybridized orbital, $\varepsilon_s^{(1)}$ and $\varepsilon_s^{(2)}$ are terms of the atoms, which have *s* electrons on the last orbital, (In Ge and Si V_0=0), *d* is the distance between atoms, *M* mass of atom. The distance between atoms insignificantly depends on the concentration of anti-bonding quasi-particles [18], but V_C and oscillation frequency depend on it significantly. If $T=0K$, $h=0$ $\omega=\omega_0$, then

$$\frac{\omega(n)}{\omega_0} = \sqrt{\frac{V_C(n)}{V_C^0}\left(\frac{1+\frac{V_0}{V_C(0)}}{1+\frac{V_0}{V_C(n)}}\right)^{3/2}}. \quad (10)$$

The probability of the fact that the atoms of the given covalent crystal will bond with each other with decreased bonding force is:

$$W_1 = \frac{\left(\frac{4\pi}{3}\left(\frac{\lambda_e}{2}\right)^3 + \frac{4\pi}{3}\left(\frac{\lambda_p}{2}\right)^3\right)n_iV}{\frac{V}{N}N} = \frac{\pi}{6}\left(\lambda_e^3 + \lambda_p^3\right)n_i \quad (11)$$

and the probability of occurrence of ordinary bonding is:

$$W_2 = 1 - W_1 = 1 - \frac{\pi}{6}\left(\lambda_e^3 + \lambda_p^3\right)n_i. \quad (12)$$

It means that

$$V_C(n) = \left(1 - \frac{\pi}{6}\left(\lambda_e^3 + \lambda_p^3\right)n_i\right)V_C^{(0)} + \frac{\pi}{6}\left(\lambda_e^3 + \lambda_p^3\right)n_iV_e^{(1)}. \quad (13)$$

As is known, in pure semiconductor:

$$n_i = n = p = \frac{\left(2\pi\sqrt{m_{de}m_{dp}}KT\right)^{3/2}}{4\pi^3\hbar^3}e^{-\frac{\varepsilon_g(T)}{2KT}} \quad (14)$$

and $\varepsilon_g(T)=\varepsilon_g(0)-\frac{\alpha T^2}{T_0+T}$ [19]; m_{de} and m_{dp} are effective masses of electrons' and holes' density. Let us say that $\gamma=1-\frac{V_C^{(1)}}{V_C^{(0)}}$;

$$\xi=\left(\frac{\left(1+\frac{V_0}{V_C^0}\right)}{\left(1+\frac{V_0}{V_C^{(n)}}\right)}\right)^{3/2}$$ and

$$\delta=\left(\frac{2\pi}{3}\right)^{3/2}\left(\frac{\pi}{3q(T_m)}\right)\left(\left(\frac{\sqrt{m_{de}m_{dp}}}{m_e}\right)^{3/2}+\left(\frac{\sqrt{m_{de}m_{dp}}}{m_p}\right)^{3/2}\right).$$

According to this we get:

$$\omega_n=\omega_0\sqrt{1-\frac{\pi}{6}\gamma\xi\left(\lambda_e^3+\lambda_p^3\right)n_i}=\omega_0\sqrt{1-\delta\gamma e^{-\frac{\varepsilon_g(T)}{2KT}}}.$$

Based on the definition of heat capacity, the equation will be:

$$C=3NK\left\{\left(\frac{\hbar\omega(n)}{KT}\right)^2\frac{e^{\frac{\hbar\omega(n)}{KT}}}{\left(e^{\frac{\hbar\omega(n)}{KT}}-1\right)^2}+\frac{1}{4}\left(\frac{\hbar\omega(n)}{KT}\right)\left(\frac{\varepsilon_g(0)}{KT}+\frac{\alpha TT_0}{K(T_0+T)}\right)\right.$$

$$\left.\frac{\delta\gamma\xi e^{-\frac{\varepsilon_g(T)}{2KT}}}{\sqrt{1-\delta\gamma\xi e^{-\frac{\varepsilon_g(T)}{2KT}}}}\left(\frac{1}{e^{\frac{\hbar\omega(n)}{KT}}-1}-\left(\frac{\hbar\omega(n)}{KT}\right)\frac{e^{\frac{\hbar\omega(n)}{KT}}}{\left(e^{\frac{\hbar\omega(n)}{KT}}-1\right)^2}\right)\right\}. \quad (15)$$

Other constants – α_1, T_0 and others for some covalent crystals are given in Table 1.

Results of this formula for Si, Ge, and GaAs are given in Fig. 5. Light dots are the experimental results for Ge [5] and black dots for Si [5].

In the case of low temperatures, when $\hbar\omega >> KT_{(n)}$, then $\omega_{(n)}H\approx\omega_0$ and Formula (15) will change like this:

$$C=3NK\left(\frac{\hbar\omega_0}{KT}\right)^2 e^{-\frac{\hbar\omega_0}{KT}}. \quad (16)$$

This result is similar to that of Einstein's theory for low temperature range. In case of high temperature, when $\hbar\omega << KT_{(n)}$, according to Formula (15) we get:

$$C=3NK\left\{1+\frac{\hbar\omega(n)}{KT}\left(1+\frac{1}{4}\left(\frac{\varepsilon_g(0)}{KT}+\frac{\alpha TT_0}{K(T+T_0)}\right)\right)\frac{\delta\gamma\xi e^{-\frac{\varepsilon_g(T)}{2KT}}}{1-\delta\gamma\xi e^{-\frac{\varepsilon_g(T)}{2KT}}}\right\} \quad (17)$$

In the case of nanostructures, these formulas work well, excepting those in which concentration of charge carriers in pure semiconductors takes place. As all parameters are same, except n_i, we get [20]: $n_i=\sqrt{N_C N_V}e^{-\frac{\varepsilon_g(T)}{2KT}}$, where $N_C^{2D}=\frac{m_{de}KT}{\pi\hbar^2W}$ and $N_V^{2D}=\frac{m_{dV}KT}{\pi\hbar^2W}$, where N_C^{2D} and N_V^{2D} are densities of quantum states at the edges of conducting and valence bands in 2D systems. W is the thickness of the sample. According to this data, the dependence between temperature and oscillation frequency is:

$$\omega(T)=\omega_0\sqrt{1-\delta_1\gamma\xi\frac{e^{-\frac{\varepsilon_g(T)}{KT}}}{W\sqrt{KT}}}. \quad (18)$$

Table 1

	$\varepsilon_g(0)(ev)$	$\alpha(ev/K)$	T$_0$,K	m_{de}/m_0	m_{dp}/m_0	m_e/m_0	m_p/m_0	$V_2^{(0)}(ev)$
Ge	0.74	$4.77\cdot10^{-4}$	235	0.57	0.37	0.18	0.25	-5.6
Si	1.17	$4.73\cdot10^{-4}$	636	1.08	0.59	0.26	0.38	-6.1
GaAs	1.519	$5.4\cdot10^{-4}$	204	0.85	0.53	0.067	0.15	-5.56

$V_2^{(1)}(ev)$	$\omega_0 c^{-1}$	$\omega_1\sec^{-1}$	$q(T_m)$	$n_i(T_m), cm^{-3}$	T_m, K	δ	γ	$C(T_m)$
-2.4	$5\cdot10^{13}$	$3.4\cdot10^{13}$	6.5	$1.84\cdot10^{19}$	1210	3.4	0.57	9.5
-2.6	$9\cdot10^{13}$	$6\cdot10^{13}$	3.66	$3.2\cdot10^{19}$	1690	7.3	0.57	10
-2.4	$4.7\cdot10^{13}$	$2.3\cdot10^{13}$	6.35	$7.4\cdot10^{18}$	1511	20.6	0.57	7.14

Where $\delta_1 = \frac{4\pi^3\sqrt{m_{de}m_{dp}}}{9\sqrt{3}q(T_m)}\left(m_e^{-\frac{3}{2}} + m_p^{-\frac{3}{2}}\right)$. The final Formula for heat capacity will be:

$$C = 3NK\left\{\left(\frac{\hbar\omega(n)}{KT}\right)^2 \frac{e^{\frac{\hbar\omega(n)}{KT}}}{\left(e^{\frac{\hbar\omega(n)}{KT}} - 1\right)^2} - \frac{1}{4}\left(\frac{\hbar\omega(n)}{KT}\right)\frac{\xi\gamma\delta_1}{\sqrt{KTW}}\left(\frac{\varepsilon_g(0)}{K_0T} + \frac{\alpha TT_0}{K(T+T_0)^2} - 1\right)\times \frac{e^{-\frac{\varepsilon_g(T)}{2KT}}}{\sqrt{1-\delta_1\gamma\xi\frac{e^{\frac{\varepsilon_g(T)}{2KT}}}{W\sqrt{KT}}}}\left(\frac{1}{e^{\frac{\hbar\omega(n)}{KT}}-1} - \left(\frac{\hbar\omega(n)}{KT}\right)\frac{e^{\frac{\hbar\omega(n)}{KT}}}{\left(e^{\frac{\hbar\omega(n)}{KT}}-1\right)^2}\right)\right\}. \quad (19)$$

In high temperature range, when $\hbar\omega >> KT$:

$$C = 3NK\left\{1 + \left(\frac{\hbar\omega(n)}{KT}\right)\left(1 + \frac{1}{4}\frac{\xi\gamma\delta_1}{\sqrt{KTW}}\left(\frac{\varepsilon_g(0)}{KT} + \frac{\alpha TT_0}{K(T+T_0)} - 1\right)\right)\frac{e^{-\frac{\varepsilon_g(T)}{2KT}}}{1 - \delta\gamma\xi\frac{e^{-\frac{\varepsilon_g(T)}{2KT}}}{\sqrt{KTW}}}\right\}. \quad (20)$$

As it seems, in the case of low temperature range in 3D systems, as well as in 2D crystals, dependence between heat capacity and temperature is described with the same equation, but in high temperature range in 2D system, besides this dependence, there appears a dependence on its nanocrystal's depth.

Let us see how our equation complies with the first principle. In our calculations we used results based on Maxwell-Boltzman's distribution functions (rules of classical statistics). We can use them if between Fermi level and corresponding band level energetic difference is $2KT \div 3KT$. We consider the semiconductors where the location of Fermi level, according to classical statistic rules is given as follows:

$$F = \frac{E_C - E_V}{2} - \frac{3}{4}KT\ln\frac{m_n}{m_p} = \frac{E_C - E_V}{2} - \Delta(T).$$

Even at the highest temperature in Ge and Si $\Delta(T_m)$~$2KT$, and $\Delta(T_m)$~$3KT$. This means that we can

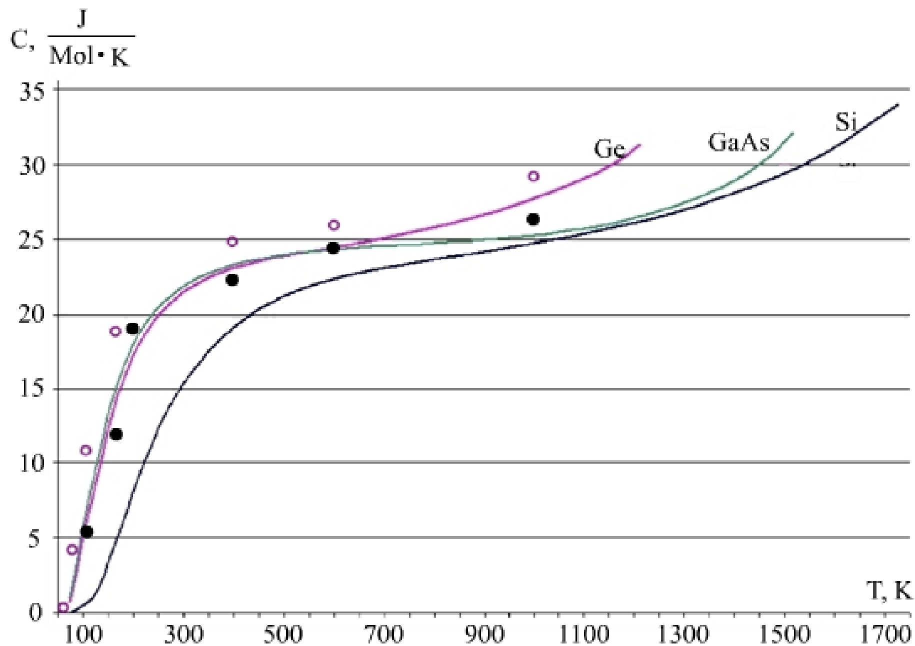

Fig. 5. Dependence between heat capacity and temperature in 3D crystals in Ge and Si according to Formula (15) [5].

use rules of classical statistics. As to using basic criteria of a kinetic equation it looks like: $E\Delta t >> \hbar \Rightarrow d >> \frac{\lambda_D}{2\pi}$, where d is the average distance between anti-bonding quasi-particles. $d \sim \frac{\lambda_D}{\sqrt[3]{q(T_m)}}$, because $\sqrt[3]{q(T_m)} \sim 1.5 \div 1.8$; $\frac{d}{\lambda_D} = \frac{2\pi}{\sqrt[3]{4}} > 1$. So, there is no strict inequality; however $\frac{d}{\lambda_D} > \pi > 1$. So, using kinetic equation criteria is met approximately.

5. Summary. The interatomic bonding energy was calculated in covalent crystals in the state of $sp^3 \rightarrow sp^2s^-$ excitement (when sp^3 bonding electron takes anti-bonding position). It is shown that part of *s* state increases and *p* state's part decreases many times in *sp³* hybrid bonding in this state. This causes an increase of the degree of freedom of atoms, so this means that the state becomes "fluid" or "soft". Besides, interatomic bonding force decreases and based on this conception, we considered the melting process and defined the critical concentration of anti-bonding quasi-particles. These anti-bonding particles form not only by heat transfer, but by any external excitement (light, injection of charge carriers, pressure etc.). The heat capacity in Einstein's solid state model is calculated according to the dependence between phonon spectrum of atoms and concentration of anti-bonding quasi-particles. These calculations are made for 3D crystals as well as for underdeveloped-dimensional nanocrystals. Calculations, performed using this method show that, as is seen in Fig. 5, in general crystals, calculated heat capacity agrees with experimental data better than the calculation results using previous methods. Our method is not very accurate but it has other positive sides: this is a methodologically new principle which can be used in the case of states with different type of chemical bonding in 3D systems, as well as in underdeveloped-dimensional systems.

ფიზიკა

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საქართველოს ტექნიკური უნივერსიტეტი

(წარმოდგენილია აკადემიის წევრის გ. ჩაგელიშვილის მიერ)

მოცემულ ნაშრომში გათვლილია sp^3 და sp^2s^- ჰიბრიდული ბმების ბმის ენერგიები. გათვლები ჩატარებულია ანტიმაკავშირებელი კვაზინაწილაკების ატომთაშორის ბმის ენერგიაზე გავლენის გათვალისწინებით (როდესაც მაკავშირებელი ნაწილაკი გადადის ანტიმაკავშირებელ მდგომარეობაში). ასევე განხილულია დნობის პროცესი კოვალენტურ კრისტალებში და განსაზღვრულია ანტიმაკავშირებელი კვაზინაწილაკების კრიტიკული კონცენტრაცია, რომელზეც იწყება დნობა და ეს შეიძლება გამოწვეული იყოს არა მხოლოდ სითბოს გადაცემით,

არამედ სხვა გზებითაც (სინათლის დასხივებით, მუხტის მატარებლების ინჟექციით და ა.შ.). ასევე გათვლილია კუთრი სითბოტევადობა მყარი სხეულის აინშტაინისეულ მოდელში როგორც სამგანზომილებიანი, ასევე ორგანზომილებიანი სისტემებისათვის.

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