CORRELATION BETWEEN MECHANICAL PROPERTIES OF DIAMOND-LIKE SEMICONDUCTOR COMPOUNDS AND LATTICE THERMAL CONDUCTIVITY

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• *Analysis is performed and mechanical (elastic) properties of semiconductor compounds of the type $A^n B^{8-n}$ (n = 1, 2, 3) possessing different chemical bond ionicity f_m are compared to their lattice thermal conductivity χ_P at T = 300 K. It is shown that with a growth in f_m and the degree of elastic anisotropy $A = 2C_{44}/(C_{11} - C_{22})$ (C_{ij} are elastic constants in Voigt notation), the values of χ_P monotonically decrease from phosphides to sulphides up to halogenides. Thus, for the first time functional dependence $\chi_P(A)$ has been established. Evaluation of technological parameters necessary in the design and manufacture of thermoelectric devices has been proposed.*

Introduction

The title of this work can arouse certain perplexity among specialists in thermoelectricity: does it make sense to analyze, compare and discuss mechanical properties and thermal conductivity χ of solids used in the calculation of thermoelectric figure of merit $Z = \alpha^2 \sigma/\chi$ (α, σ are the Seebeck coefficient and electroconductivity)? Really, considering the Seebeck, Justi and Meissner series, it is easy to see that metals possessing high values of σ, χ and mechanical properties (elastic constants C_{ijkl}, Young's, shear and compression moduli, etc) are characterized by essentially lower Z values as compared to semimetals and semiconductors (see, for instance, [1]).

However, in the selection of a specific thermoelectric material (for any application area) the question of one-to-one correspondence between mechanical, thermal and thermoelectric properties should be solved by taking into account all real factors assuring both mechanical stability and high Z values over wide ranges of temperature and pressure. Below are given the analysis and the respective calculation procedure as applied to binary semiconductor compounds of the type $A^n B^{8-n}$ ($n = 1, 2, 3$). Selection of these materials is due to the fact that they are characterized by different chemical bond ionicity f_m affecting considerably both equilibrium (mechanical, thermal, caloric) and non-equilibrium (lattice thermal conductivity, internal friction, viscosity) properties, and, particularly, electrophysical properties. As was emphasized in [2], mechanical characteristics, such as hardness, brittleness and plasticity are no less important than thermoelectric properties of this material to assure high reliability of respective products, instruments and devices.

In retrospect, attention should be paid to the circumstances that played an important role in the understanding and interpretation of the scientific and applied aspects of thermoelectric instrument making.

As the area of research on the physical properties is expanded from the elementary semiconductors *Ge, Si, β-Sn* to their binary analogs – $A^n B^{8-n}$ ($n = 1, 2, 3$) compounds, not only crystal structure has changed (for instance, the inversion centre has disappeared), but also a qualitatively new type of chemical bond-mixed ion-covalent – has been formed due to interaction between two sorts of atoms in the respective sites of diamond-type crystal lattice. Besides, the difference in their band structure, i.e. energy spectra $\varepsilon(\vec{p})$ (ε is energy, $\vec{p}$ is quasi-pulse) have led to considerable changes in

the electrical, magnetic, optical, thermoelectric and thermomagnetic properties. It is appropriate to emphasize that unlike the electrophysical properties, the mechanical and thermal properties of the above compounds have not been properly subject to quantitative analysis up to the present time, and only in a recent paper [3] the influence of ionicity f_m of $A^n B^{8-n}$ (n = 1, 2, 3) compounds on their elastic properties was quantitatively estimated. Thus, the purpose of this work is as follows:

I. To establish quantitative correlation between the mechanical properties of $A^n B^{8-n}$ (n = 1, 2, 3) compounds and their lattice thermal conductivity χ_P.

II. Based on item I, to propose a procedure for estimation of the mechanical properties of thermoelectric materials subject to thermomechanical treatment, needed both in the design and manufacture of high-figure-of-merit devices possessing proper mechanical stability.

Physical interpretation of a correlation between mechanical (elastic) properties and lattice thermal conductivity χ_P

The fundamental relationship obtained in the historically first theory of thermal conductivity of dielectric solids proposed by P. Debye [4] is as follows:

$$\chi_p = \frac{1}{3} C_V \overline{\upsilon} \overline{l}, \tag{1}$$

where C_V is heat capacity of substance volume unit, $\overline{\upsilon}$ is the average speed of sound waves propagation, $\overline{l}$ is their mean free path.

In the Debye approximation, crystal lattice is considered as a continuous elastic medium (the so-called elastic continuum) where longitudinal and transverse acoustic vibrations can propagate with different frequencies ω linearly dependent on the wave vector $\vec{q} = \frac{2\pi}{\lambda} \vec{n}_0$ (λ is wavelength). It means that vibration dispersion $\omega(\vec{q})$ is not taken into account, owing to which the group and phase velocities of elastic waves coincide.

Nevertheless, the atomic structure according to P.Debye is taken into account by introducing the restricting (maximum) frequency $\omega_{max} = \omega_D$ (the so-called Debye frequency). The latter is determined from the condition of retention of the number of degrees of freedom *3N* (*N* is Avogadro constant) – normalization condition:

$$3N = A \int_0^{\omega_D} f_D(\omega) d\omega, \tag{2}$$

where *A* is a constant appearing in the expression for the Debye function of frequency spectral distribution $f_D = A \cdot \omega^2$, i.e. the number of vibrations found in the frequency range $[\omega, \omega + d\omega]$ ($0 \le \omega \le \omega_{max} \equiv \omega_D$). Thus, *A* is determined unambiguously:

$$3N = A \int_0^{\omega_D} \omega^2 d\omega = \frac{A \omega_D^3}{3}, $$

whence

$$A = \frac{9N}{\omega_D^3} \equiv \frac{9N}{\omega_{max}^3}. \tag{3}$$

As a rule, maximum frequency $\omega_{max} \equiv \omega_D$ is represented by introducing the Debye characteristic temperature θ_D determined as

$$\theta_D = \frac{\hbar}{k}\omega_{\max} \equiv \frac{\hbar}{k}\omega_D, \tag{4}$$

where $\hbar$ and k are the Planck and Boltzmann constants.

From (4) it follows that θ_D has the dimension of temperature (K), owing to which its physical meaning becomes sufficiently transparent: θ_D is an interface between classical temperature region $T > \theta_D$, where quantization of lattice vibrations is inessential and quantum temperature region, $T < \theta_D$, where quantization of lattice vibrations is essential and considerable in the calculations of thermal equilibrium and nonequilibrium properties of solids – dielectrics, semiconductors, semimetals and metals [*].

Coming back to equation (1), one can trace a correlation between χ_P and the elastic properties of a substance. Really, according to classical theory of elasticity the values of Young's modulus E, shear modulus G, compression modulus B of solid body are proportional to squared velocity of propagation of sound waves of different polarization (longitudinal, transverse, mixed): $E \sim \rho \upsilon^2_{long}$, $G \sim \rho \upsilon^2_{trans}$, etc. Hence, the higher are the absolute values E, G, B of the medium, the higher are χ_P values. Moreover, based on relationship (1) one can explain even the temperature dependence $\chi(T) \sim 1/T$ in classical region $T > \theta_D$.

Further progress in P.Debye's theory of thermal conductivity is related to the names of famous physicists R. Peierls, G. Leibfried, J. Ziman et al [4].

Using the atomistic models of crystal lattices, with regard to different types of interactions between atoms (molecules), dependences $\chi_P(T)$ were obtained in wide temperature ranges $T \gtrless \theta_D$. The above dependences are given in the well-known monographs [4, 6]. According to [7], the most acceptable for applied calculations in cubic syngony crystals is Leibfried-Shlemann ratio in the region $T > \theta_D$:

$$\chi_P(T) = \frac{12}{5}\sqrt[3]{4}\left(\frac{k}{\hbar}\right)^3 M\delta\theta_D^3 \Big/ \gamma_G^2 T, \tag{5}$$

where M is atom mass, δ^3 is volume per one atoms, γ_G is Gruneisen parameter taking into account changes in lattice vibration frequencies due to volumetric thermal expansion [**]

$$\gamma_G = -d\ln\theta_D \Big/ d\ln V > 0. \tag{6}$$

It is important to emphasize that thermodynamic parameter γ_G can be calculated using the data measured experimentally:

$$\gamma_G = \frac{\beta}{\kappa}\frac{V}{C_V}, \tag{7}$$

where β is coefficient of volumetric expansion, κ is volumetric compressibility, C_V is lattice heat capacity of substance gram-atom[***]. For the estimation of many lattice properties of crystals the average value $\langle\gamma_G\rangle \simeq 2$ is assumed (though for covalent crystals $\gamma_G = (0.50 \div 0.75)$), and for quantum and cryocrystals $\gamma_G = 3$ [11]). In conformity with expression (5), a correlation between $\chi_P(T)$ and the

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[*] The gnoseological importance of θ_D (determined by various physical methods) as an attribute of modern solid state physics, see for instance, in recent work [5].
[**] In the general case for crystals of any symmetry the values θ_D and γ_G form a symmetrical second-rank tensor, namely: the Debye frequency tensor [8] and the Gruneisen tensor [9].
[***] The values γ_G can be also determined from the data of temperature attenuation of X-ray diffraction intensities, from the data of compressibility dependences on pressure, the Hugoniot adiabats, from the data of powerful laser radiation absorbed by crystal in pulsed mode with a constant volume [10]

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elastic properties of crystals lies in the possibility of calculating θ_D from the experimental data of components of elastic constant tensor C_{ijkl} (fourth rank), appearing in the generalized Hooke's law establishing a linear relationship between stress tensor σ_{ij} and deformation tensor ε_{kl}. The thus calculated $\theta_D^{(elast)}$ coincides with the value $\theta_D^{(c)}$, determined from the data of temperature dependence of lattice heat capacity $C_V(T)$ in the cryogenic temperature region of the order $\theta_D/100$, where the true P. Debye's law $C_V \sim T^3$ is fulfilled.

Thus, from the above considered physical reasoning for a relation between the mechanical and thermal properties of nonmetal crystals one can draw a unique conclusion, namely: the higher is the absolute value of components of elastic constant tensor, Debye frequency tensor, and the lower are the absolute values of Gruneisen tensor components[*), the higher is thermal conductivity of this crystals, irrespective of crystal syngony.

For instance, a diamond possessing "record" value $\theta_D \approx 2000$ K among the non-conducting crystals is characterized by the highest value of χ_P which exceeds $2 \div 5$ times the thermal conductivity of Cu and Ag – the best heat conductors.

We emphasize that with the physical substantiation of a correlation between the mechanical properties and χ_P of semiconductor alloys of the type *Ge-Si*, diamond-like compounds of the type A^nB^{8-n} ($n = 1, 2, 3$), intermetallic compounds (doped and undoped), as well as other thermoelectric materials, the information on the character of chemical bond, i.e. distribution of electron density $\rho(x)$ in these unit cells, is necessary and vital.

Theoretical calculations of $\rho(x)$ (band structure) are covered in scientific literature in sufficient detail (see, for instance, [12]). Experimental determination of $\rho(x)$ is generally based on the data of analysis of the intensities of *X*-ray diffractions and determination of Fourier-components of structural factor (the so-called F^2 of the body [13]).

Nevertheless, the ionicity of mixed ion-covalent bond of diamond-like semiconductor compounds A^nB^{8-n} ($n = 1, 2, 3$) with a sufficient degree of accuracy can be determined by the deviation from M.Born ratio for the elastic constants C_{ij} of these compounds, as is shown in [14, 15]:

$$f_m = 1 - \Lambda, \tag{8}$$

where

$$\Lambda = \frac{4C_{11}(C_{11} - C_{12})}{(C_{11} + C_{12})^2}. \tag{9}$$

(C_{ij} is in Voigt notation).

Note that C_{ij} can be used for the calculation of rather important in application sense elastic characteristics, such as Young's modulus E, torsion modulus G (depending on the direction in crystal). Besides, of no less importance physically are elastic parameters (not dependent on direction in crystal) determined from the data of C_{ij}, namely:

compression modulus:

$$B = \frac{(C_{11} + 2C_{12})}{3} \tag{10}$$

and elastic anisotropy factor

[*) In some crystals with different character of chemical bond the so-called modal components of the Gruneisen tensor γ_i can be negative. However, the latter factor does not affect the sign of χ_P, as it is seen from Eq. (5).

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \qquad (11)$$

(the so-called A-factor) the physical meaning of which is sufficiently transparent. The value B to a certain degree reflects the energy of interatomic (intermolecular, interionic) repulsion, and A-factor is a measure of relative resistance of crystal lattice to two types of shear deformation: C_{44} characterizes shear resistance in plane (010) in direction [001], and $(C_{11} - C_{12})/2$ – shear resistance in plane (110) in direction [$\bar{1}$10]. Exactly for this reason A-factor is used for the interpretation of chemical bond rigidity and interatomic interactions. In particular, for binary diamond-like compounds of the type $A^n B^{8-n}$ ($n = 1, 2, 3$) a distinct quantitative correlation was established between A-factor and bond ionicity f_m in recent paper [3], namely: A-factor is a monotonously increasing function of f_m, and in the limiting case of purely covalent bond (diamond, $f_m = 0$) there is shown a fundamental infeasibility of $A^n B^{8-n}$ ($n = 1, 2, 3$) compounds possessing $A \leq 0.12$.

The influence of chemical bond ionicity f_m and A-factor on the lattice thermal conductivity χ_P

From the standpoint of modern solid state physics, thermal conductivity χ_P is caused by the anharmonicity of lattice thermal vibrations. The most general manifestation of anharmonicity lies in the disturbance of dynamic dependence of vibrational modes, i.e. (in terms of quantum mechanics) phonon-phonon interaction (the so-called N- and U-processes [4]). Exactly due to U-processes (carry-over processes from German "Umklapp"), the lattice thermal conductivity is a finite value (rather than infinite, like in a "harmonic" crystal). By the way, a "harmonic" crystal cannot be a thermoelectric in principle ($Z = 0$!). As long as thermal conductivity of any crystal solid depends both on the type (character) of chemical bond (band structure) and temperature, for the analysis of dependences $\chi_P(T)$ three typical temperature regions are considered:

a) high temperature region $T > \theta_D$, in which $\chi_P(T) \sim 1/T_0$.

b) low temperature region $T < \theta_D$, in which $\chi_P(T) \sim \exp(\theta_D/\xi T)$, where $1.5 \leq \xi \leq 2$ depending on chemical bond type.

c) cryogenic temperature region $T \ll \theta_D$, $\chi_P(T) \sim C_v(T)$, and phonon mean free path $l_{ph} \simeq L$, where L is macroscopic size of sample (the so-called Casimir effect [4]).

In the temperature region (b) and (c), apart from the ionicity and anharmonicity, χ_P is essentially affected by the defects of real crystal structure of solid – point, linear and plane ones [16].

In the present paper for the analysis of χ_P depending on f_m and A-factor we will restrict ourselves to region (a), where the influence of defects on χ_P is not dominant. Moreover, the region (a) $T > \theta_D$, as a rule, corresponds to temperatures that are operating for the majority of thermoelectric products and devices [1]. To discover the expected correlation between f_m, A-factor and lattice thermal conductivity χ_P, the experimental data C_{ij} are used and A-factors are given in Table I of the recent work of the author's recent work [3], and the values of χ_P at $T \geq \theta_D$ are borrowed from handbooks [17, 18].

Compounds $A^n B^{8-n}$ were chosen pairwise with a minimum difference in the ionicity f_m, in order to trace the "resolution" in the estimates of χ_P.

Apart from the above, Table 1 also shows the average values of mass $<m> = (m_1 + m_2)/2$, specific volumes V and densities ρ that will be needed for further discussion of the results.

Analyzing the data of Table 1 by the increasing ionicity f_m (from top downwards), one can be certain that there is a distinct correlation not only between f_m and A-factor, but also between f_m and χ_P: with a decrease in the bond rigidity (i.e. increase in the ionicity f_m and A-factor) there is a systematic

reduction of lattice thermal conductivity χ_P from phosphides (minimum values of χ_P and A), sulphides (intermediate values of χ_P and A) up to halogenides possessing the largest ionicity f_m and A-factor. However, for *CuI* the experimental value χ_P is unknown to us and for this reason its estimation was made by interpolation on the scale of χ_P (marked by asterisk). It can be assumed that with such interpolation we are not much mistaken, since the established regularity $f_m(\chi_P)$ is quite valid, which is independently confirmed by a reduction in χ_P with a growth in specific volume V (i.e. reduction of bond rigidity).

Table 1

Compound type	$<m>$, g	ρ, g/cm^3	V, cm^3/g·at	f_m	A	χ_P, W/cm·K	Remarks
A^3B^5 *AlP*	46.4	2.85	10.2	0.033	1.78	0.900	$T = 300$ K
GaP	80.8	4.40	11.5	0.046	1.81	0.770	
A^2B^6 *ZnS*	77.9	4.10	12.0	0.171	2.34	0.026	
CdS	115.2	4.82	14.0	0.181	2.70	0.020	
A^1B^7 *CuI*	152.0	5.63	16.9	0.207	3.16	0.0161*	Interpolations
CuBr	115.6	4.72	15.2	0.440	6.00	0.013	$T = 300$ K

Note that for the majority of semiconductor crystals the contribution to total thermal conductivity of carriers (electrons or holes) is, as a rule, insignificant [4], though for some compounds with a high thermoelectric figure of merit (such as Bi_2Te_3) the above contribution is essential.

From the standpoint of general physics, the established regularity $f_m(\chi_P)$ is quite natural: from relationship (1) it follows that the higher is the rate of sound waves propagation in given crystal due to bond rigidity, the higher is its lattice thermal conductivity (which has been well known before). The novelty of the present work is the conclusion: lattice thermal conductivity of semiconductor compounds of the type A^nB^{8-n} ($n = 1, 2, 3$) is a monotonically decreasing function of elastic anisotropy factor (A-factor) of crystal solids.

The influence of Debye temperature θ_D on lattice thermal conductivity in high-temperature region

Physical interpretation of dependences of the type $\theta_D(\chi_P)$ should proceed from the fact that the Debye temperature θ_D, apart from its general physical significance, can be considered as a measure of bond rigidity in a vibrating crystal lattice. This subject was widely discussed in due time at the All-Union conferences on the application of *X*-ray diffraction and in physics periodicals (see, for instance references in [19]). In due time the author of the present work showed that θ_D determined from *X*-ray data can be considered as a degree of bond rigidity $f \sim m \cdot \theta_D^2$ of vibrating lattice with central and noncentral interactions of the nearest and second nearest neighbours [20].

Thus, the concept "bond rigidity – lattice thermal conductivity" can be analyzed for compounds A^nB^{8-n} ($n = 1, 2, 3$) whose θ_D values are known, or can be calculated from the experimental data on the components of elastic constant tensor C_{ijkl}.

Based on the reasoning stated in the previous paragraphs of the present work, it can be expected that the regularities established for compounds A^nB^{8-n}, namely $f_m(\chi_P)$ and $A(\chi_P)$, will be also adequately reflected in the dependences $\theta_D(\chi_P)$ of the above compounds. At the same time, it should be noted that it has been well known earlier that in the high-temperature region $\chi_P \sim \theta_D^3/T$ (see formula 5). However, neither of publications referring to estimates of χ_P, interpreted the value θ_D as a measure of chemical bond rigidity. Therefore, establishment of regularities $\theta_D(\chi_P)$ on the basis of experimental

data can serve as independent additional argumentation of the fact that characteristic Debye temperature θ_D is really the measure of chemical bond rigidity in solids.

Remind that in the calculation of θ_D by the elastic constants C_{ij}, it is necessary to calculate the average sound velocity which depends both on the type of crystallographic syngony and the degree of elastic anisotropy. As is shown by the author in [5] for crystals of cubic symmetry at $A \leq 2.36$, the values θ_D are calculated by relatively simple formula:

$$\theta_D^{-3} = \frac{k_B m}{18\pi^2 h^3} \rho^{3/2} \left[\left(\frac{1}{C_{11}} \right)^{3/2} + \left(\frac{2}{C_{11} - C_{12}} \right)^{3/2} + \left(\frac{1}{C_{44}} \right)^{3/2} \right], \qquad (12)$$

where C_{ij} is in Voigt notation, the rest are generally accepted designations. Nevertheless, for crystals possessing $A \geq 2.36$ more precise are Betts formulae and others [21], where six directions of sound velocity averaging are taken into account:

$$\theta_D = \frac{h}{k_B} \left(\frac{9N}{4\pi V} \right)^{1/3} \rho^{-1/2} J_i^{-1/3}, \qquad (13)$$

N is Avogadro number, and the values J_i are combinations of C_{ij} which are not given here because of their awkwardness[*)].

In Table 2 are listed the values θ_D, calculated at $T = 300$ K by (12) from the data of C_{ij}, Table 1 of Ref. [3], and the respective χ_P, bond rigidity $<m>\theta_D^2$ and average mass value $<m>$. The values θ_D proved to be almost coincident with those determined from the heat capacity data according to handbook [18].

Table 2

Compound, type		$<m>$, g	θ_D (K)	$<m>\theta_D^2 \times 10$ dyne/cm	χ_P, W/cm·K	Remarks
A^3B^5	AlP	46.4	588	2.71	0.90	For all compounds it is assumed that $<\gamma_G> = 1$ at $T = 300$ K
	GaP	80.8	446	1.62	0.77	
A^2B^6	ZnS	77.9	310	0.76	0.026	
	CdS	115.2	260	0.73	0.020	
A^1B^7	CuI	152.0	178	0.49	0.016	
	CuBr	115.6	154	0.28	0.013	

From the table it follows that for all types of compounds A^nB^{8-n} ($n = 1, 2, 3$) with a reduction in bond rigidity $f \sim m \cdot \theta_D^2$ the lattice thermal conductivity is logically reduced, and in conformity with formula (5) the regularity of χ_P increase with a growth in θ_D is retained. Certain influence on the dependence $\chi_P(\theta_D)$ can be produced by a small difference in Gruneisen parameters γ_G which for purely covalent crystals make the value $\gamma_G = 0.75$ [11].

Thus, from the data in Tables 1 and 2 one can arrive at unambiguous assertion that characteristic Debye temperature θ_D is really a measure of chemical bond rigidity irrespective of crystallographic syngony and the type of Bravais lattices.

Some practical recommendations

Analysis of the elastic properties of compounds A^nB^{8-n} ($n = 1, 2, 3$) and their correlation to thermal conductivity allows recommending some technological parameters of these materials, such as hardness,

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[*)] The difference in θ_D values calculated by (12) and (13) is $\sim 10\%$ at $A \geq 2.36$ [5].

brittleness, plasticity. Really, when selecting a material with minimum values of χ_P to assure high values of thermoelectric figure of merit $Z \sim 1 / \chi_P$, in the design and manufacture of instruments or devices one will also require minimum hardness, minimum brittleness and maximum plasticity of chosen materials. From the data in Tables 1 and 2 it follows that minimum values of χ_P refer to A^1B^7 compounds. As regards their strength properties, it is necessary to take into account the ratio from recent work [3] relating the elastic and plastic properties:

1) plastic deformation resistance τ_P is proportional to shear modulus G and Burgers vector $\vec{b}$,

$\tau_P = G \cdot \vec{b}$

2) tear strength τ_T is proportional to compression modulus B and lattice period (specific volume V): $\tau_D = B \cdot V$

3) B/G ratio as the indicator of plasticity and brittleness: high B/G values characterize material plasticity, and low – its brittleness, namely: if $B/G < 1.75$, the material is known to be brittle.

From the data in Tables 1 and 2 it follows that maximum value $\tau_P \sim G \cdot \vec{b}$ corresponds to *AlP* compound, and minimum τ_P corresponds to *CuBr*. For the same compounds there are also extreme values of tear strength τ_T – max $(B \cdot V)$ for *InP* and min $(B \cdot V)$ for *CuBr*. As regards the B/G ratio, according to Tables 1 and 2 max $(B/G) = 5.32$ for *CuBr* and min $(B/G) = 1.57$ for *AlP*, i.e. the most brittle compounds have a low bond ionicity f_m and the most plastic ones – high value of f_m, which is quite natural.

Procedure for precise evaluation of hardness H of A^nB^{8-n} compounds was discussed in recent paper [3]. In the zero approximation, an estimate of H is permitted with respect to diamond ($f_m = 0$) by the ratio of compression moduli $B_{diamond}/B_{compound}$. Using the experimental data $B_{diamond} = 630$ GPa [22] and the respective compounds in Tables 1 and 2, we obtained $H_{GaP} = 19.6$ GPa and $H_{CuI} = 7.4$ GPa, that is the regularity $H(f_m)$ is quite natural: the value of hardness is always higher in crystals with rigid bonds (see also $f = <m> \cdot \theta_D^2$ for *GaP* and *CuI*). As applied to technological processes of hot pressing and extrusion, alongside with low values of χ_P there is also a need in high plasticity and low values of brittleness and hardness.

Conclusions

1. In the analysis of a relation between the mechanical properties of semiconductor compounds of the type A^nB^{8-n} ($n = 1, 2, 3$) to their thermal conductivity χ_P it has been first shown that the value of χ_P unambiguously depends on the degree of elastic anisotropy (*A*-factor).
2. It has been established that with a growth in *A*-factor, dependence $\chi_P(A)$ is a monotonically decreasing function at $T = 300$ K.
3. It has been shown that with a growth in θ_D, dependence $\chi_P(\theta_D)$ is a monotonically increasing function of θ_D, thus confirming that $f = <m> \cdot \theta_D^2$ is a degree of chemical bond rigidity in a vibrating lattice of crystalline solids, irrespective of the type of crystallographic syngony.

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