
CORRELATION BETWEEN THE THERMAL PRESSURE AND THE ISOCHORIC HEAT CONDUCTIVITY OF SOLID CO₂ AND NH₃

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The analysis of the correlation between the thermal pressure and the isochoric heat conductivity of solid CO₂ and NH₃ has been carried out. The temperature dependences of the thermal pressure and the isochoric heat conductivity for specimens with various molar volumes have been obtained. The isothermal dependences of the heat conductivity of solid CO₂ and NH₃ on the pressure have been calculated. The form of the temperature dependence of the isochoric heat conductivity taking the thermal pressure into account has been revealed. It has been established that the temperature behavior of the isochoric heat conductivity of solid CO₂ and NH₃ is governed by the phonon-phonon interaction and the additional influence of the thermal pressure.

1. Introduction

According to the theory of three-phonon scattering [1], the phonon contribution to the heat conductivity of dielectric crystals λ at the temperatures T of the order of or higher than the Debye one ($T \geq \Theta_D$) must decrease in accordance with the law $\lambda = f(1/T)$ as the temperature grows. But as early as in the first experimental works dealing with the study of heat conduction in molecular crystals, the results that cannot be described in the framework of classical theoretical models of heat transfer were obtained [1]. Both the isobaric and isochoric heat conductivities of molecular crystals possess the temperature dependences that differ essentially from the dependence $\lambda \propto 1/T$ which is characteristic of the mentioned temperature range. As was shown by Clayton and Batchelder [2], deviations of the heat conductivity from the law $1/T$ in the isobaric case are caused first of all by processes connected to thermal expansion of specimens under study. On the other hand, deviations of the isochoric heat conductivity from the

dependence $1/T$ are connected to the availability of additional, as compared to atomic crystals, types of thermal motion of molecules in molecular crystals, which are capable to affect the temperature dependence of the heat conductivity, in particular, the orientational motion of molecules at the sites of the crystal lattice [3–5].

If the noncentral interaction forces in a substance are relatively insignificant and the temperature is sufficiently high, then the molecules of such a substance possess significant orientational mobility. In a specific substance and at a certain temperature, the character of the orientational motion of molecules can change from librations and insignificant reorientations in orientationally ordered phases to practically free rotations in orientationally disordered ones. The transition of molecules to the permanent rotation, as the temperature grows, is accompanied by an increase of the isochoric heat conductivity [6, 7]. A contribution of the rotational motion of molecules to the heat conduction is minor owing to a low group velocity of librations, while the scattering of phonons by rotational excitations of the crystal lattice may be comparable with that by phonons. In the case where the reduction of phonon-rotational thermal resistance, caused by the gradual transition of molecules to the decelerated rotation, exceeds the increment of the thermal resistance connected to the phonon-phonon interaction, the total heat conduction increases with the temperature. But it should be noted that the dependence weaker than $\lambda \propto 1/T$ is also observed in the crystals of inert gases, which are characterized by the absence of orientational motion, and in some molecular crystals which consist of highly asymmetric

molecules and where the orientational ordering in the solid phase always exists [8,9]. This circumstance means that the deviations of the isochoric heat conductivity in the considered case from the classical dependence $1/T$ cannot be explained only by the influence of the phonon-rotational interaction. In work [10], the model for the description of the behavior of the isochoric heat conductivity of molecular crystals in orientationally ordered phases was proposed. This model assumed that heat is transferred by low-frequency phonons and “diffusive” modes migrating randomly from site to site. Two fitting parameters were used in calculations; their values were determined according to the criterion of the minimal heat conduction.

As was already mentioned, the processes connected to the thermal expansion of specimens under consideration affect the behavior of the temperature dependence of the isobaric heat conductivity. Therefore, to make the comparison of the experimental results with the theoretical prediction as correct as possible, the comparison must be done at constant volume to exclude the influence of thermal expansion. At the same time, when carrying out the isochoric experiment under the condition that the temperature rises, the measuring ampoule of practically constant volume prevents the specimen from thermal expansion, which results in the increase of thermal pressure in the studied crystal structures [11, 12]. This factor can influence the thermophysical properties of the crystals under consideration, in particular, the heat conductivity. In this work, the analysis of the correlation between thermal pressure, which arises in the specimens under investigation, and isochoric heat conductivity has been carried out. Solid CO_2 and NH_3 served as examples. Such an analysis has not been done until now, and thermal pressure was considered to possess no essential influence on isochoric heat conductivity.

2. Results and Their Discussion

CO_2 and NH_3 possess rather wide temperature intervals of existence in a solid phase, their melting temperatures T_m being 216.6 and 195.4 K, respectively [1]. The structural researches [1, 13] established that solid CO_2 and NH_3 exist only in a single crystal modification at the corresponding pressures of their own saturated vapors. Solid CO_2 belongs to crystals made up of linear molecules. It has the fcc structure of the $Pa3$ spatial symmetry, with four molecules per elementary cell oriented along the spatial diagonal of the cube [14]. A strong noncentral interaction in crystalline CO_2 is

caused mainly by the quadrupole-quadrupole interaction and allows the orientational ordering to be preserved up to the melting temperature [15]. The entropy of melting $\Delta S = 9.23 \text{ cal}/(\text{mol} \cdot \text{K})$ of crystalline CO_2 is rather high because the translational and orientational orders are destroyed simultaneously when the crystal melts [13]. Solid NH_3 is composed of molecules which are more complex and have the form of a regular pyramid. It has the fcc structure of the $P2_13$ spatial symmetry, with the third-order axes oriented along the diagonals of the cube [16]. An elementary cell contains four molecules, the centers of mass of which are positioned at the sites of the crystal lattice. The noncentral part of the intermolecular interaction stems mainly from the dipole-dipole interaction and the hydrogen bond. It is so substantial that the orientational ordering in solid NH_3 persists up to the melting temperature [17]. The values of the characteristic Debye temperature of CO_2 and NH_3 are well below the corresponding temperatures of the phase transition and are equal to 128 and 120.1 K, respectively [1].

For today, the results of experimental researches of the isobaric λ_P and isochoric λ_V heat conductivities of solid CO_2 and NH_3 are known [18–21]. The isobaric and isochoric heat conductivities of crystalline CO_2 and NH_3 have the temperature dependences that differ from the classical law $1/T$ [1].

The results of experimental studies of the isochoric heat conductivity of solid CO_2 for specimens with the molar volume $V_{\text{mol}} = 25.85 \text{ cm}^3/\text{mol}$ and the values of the isochoric heat conductivity of solid NH_3 , which were calculated according to formula (2), for specimens with the molar volume $V_{\text{mol}} = 19.45 \text{ cm}^3/\text{mol}$ are presented in Fig. 1. The eligibility of applying formula (2) for recalculating the values of the isobaric heat conductivity to a constant density is confirmed by a good agreement between the results of similar calculations and direct experimental measurements of the isochoric heat conductivity of other molecular crystals [4–12].

The temperature dependences of the thermal pressure P that arises in the specimens of solid CO_2 and NH_3 upon isochoric researches (Fig. 2) were obtained making use of formula [9]

$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{\gamma C_V}{V_{\text{mol}}}, \quad (1)$$

where γ is the Grüneisen parameter (see Table 2), C_V is the isochoric heat capacity, and V_{mol} is the molar volume. The data of works [1, 17, 21] were used in calculations. As is seen from Fig. 2, the thermal pressure grows with temperature in the isochoric specimens. In

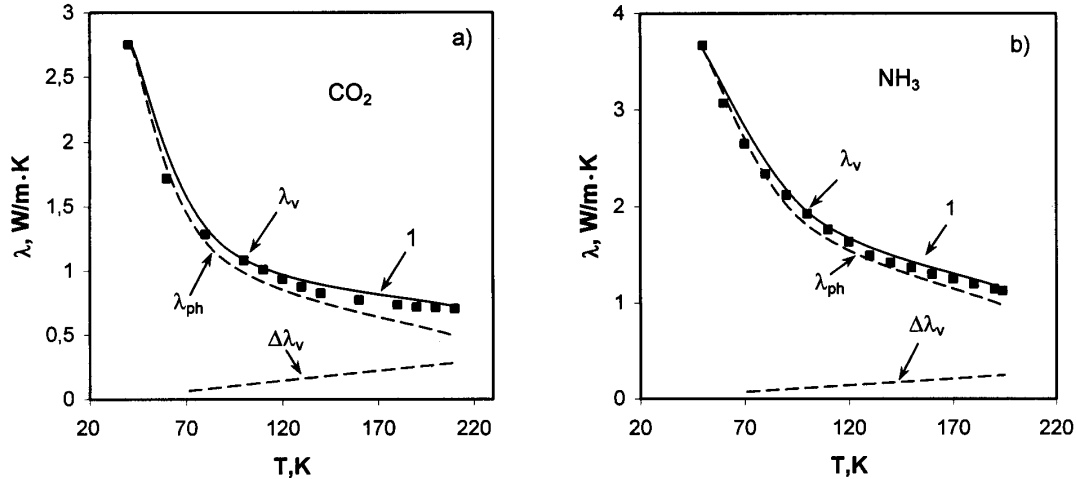


Fig. 1. Temperature dependences of the isochoric heat conductivity λ_V (squares) and the results of calculations of the phonon contribution λ_{ph} and the additional contribution of thermal pressure $\Delta\lambda_V$ to the isochoric heat conductivity for specimens of solid CO₂ with the molar volume $V_{mol} = 25.85 \text{ cm}^3/\text{mol}$ (a) and solid NH₃ with the molar volume $V_{mol} = 19.45 \text{ cm}^3/\text{mol}$ (b). Curves 1 correspond to the heat conductivity calculated according formula (8)

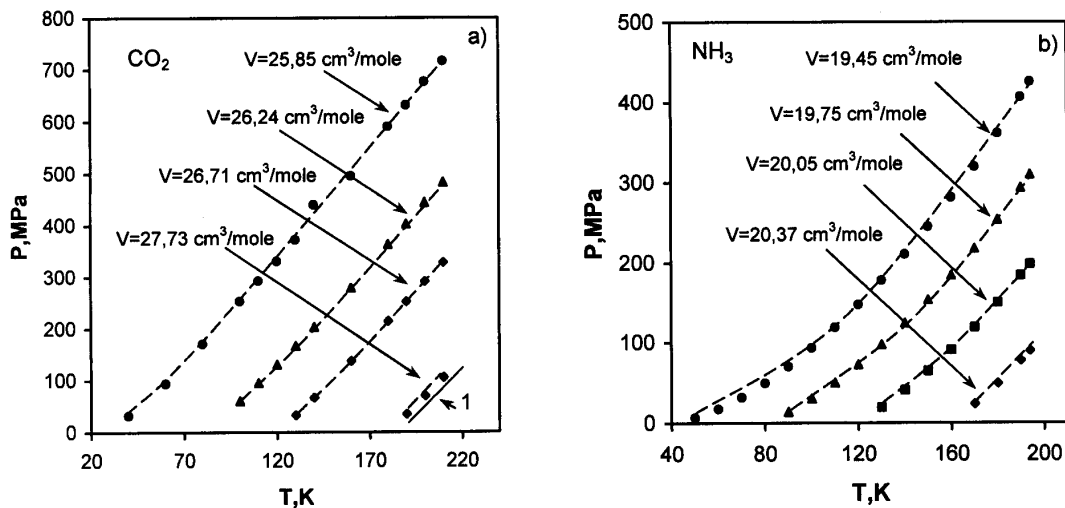


Fig. 2. Temperature dependences of the thermal pressure for specimens of solid CO₂ (a) and NH₃ (b) with various molar volumes. Curve 1(a) corresponds to experimental data [12]

the specimens of solid NH₃ with the molar volume $V_{mol} = 19.45 \text{ cm}^3/\text{mol}$, the thermal pressure grows by more than three orders of magnitude, and in the specimens of solid CO₂ with the molar volume $V_{mol} = 25.85 \text{ cm}^3/\text{mol}$ by almost four orders of magnitude. The values of the molar volume (Fig. 2) depend on the specimen growing temperature. The results of calculations agree well with the data of direct studies of thermal pressure in solid CO₂ [19] which are obtained for the specimens with the molar volume $V_{mol} = 27.78 \text{ cm}^3/\text{mol}$ and presented in Fig. 2 by a solid curve 1.

The temperature dependences of the isochoric heat conductivity λ_V (Fig. 3) for the specimens of solid CO₂ and NH₃ with various molar volumes (these dependences are needed afterwards to obtain the dependence of the isothermal heat conductivity on pressure, $\lambda_T(P)$) were calculated according to the formula [11]

$$\lambda_V = \lambda_P \left(\frac{V_{mol}(T)}{V_{m0}} \right)^g, \quad (2)$$

where $V_{mol}(T)$ is the molar volume of a free specimen as a function of temperature, V_{m0} is the recalculated molar

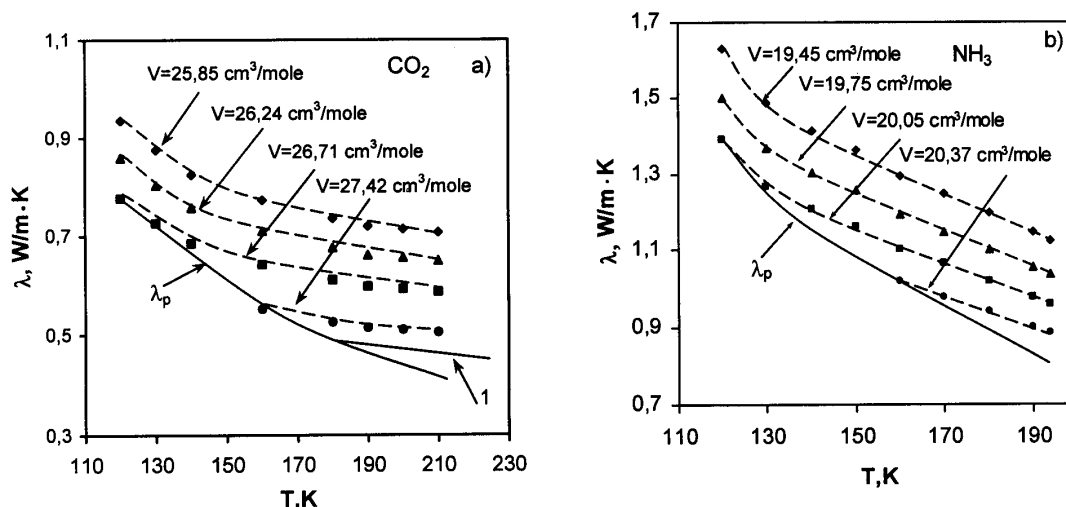


Fig. 3. Temperature dependences of the isochoric heat conductivity of solid CO_2 (a) and NH_3 (b) with various molar volumes. Curve 1 corresponds to the data of direct measurements of the isochoric heat conductivity [12]

volume of the specimen, and $g = -(\partial \ln \lambda / \partial \ln V)_T$ is the Bridgman factor. The value of the Bridgman factor for solid NH_3 (table 2) was calculated according to the formula $g = 3\gamma + 2q - 1/3$ [10]. At temperatures of the order of and above the Debye one, it is usually admitted that $\gamma \sim V$ and the second Grüneisen coefficient $q \approx 1$ [22]. According to the data of work [10], the Bridgman factor was accepted to be 5.7 for solid CO_2 .

Molecular crystals are characterized by large coefficients of thermal expansion. Therefore, in the course of isochoric experiments, an increase of thermal pressure occurs in specimens as the temperature grows [9,11]. A crystalline specimen with a constant density undergoes the action of the constantly increasing pressure creating by a measuring ampoule, the material of which has the coefficient of thermal expansion smaller by several orders of magnitude than those of molecular crystals.

The calculations carried out according formula (2) showed (Fig. 3) that the isochoric heat conductivity at a given constant temperature has different values which depend on the molar volume of the crystal. This dependence can be explained by the influence of thermal pressure which increases in the studied specimens proportionally to the increase of the temperature interval, where the condition that the experiment is isochoric holds true. The last is confirmed by both straightforward calculations (Fig. 2) and direct measurements of the dependence of heat conductivity on pressure, e.g., for solid C_6H_6 and CCl_4 [23, 24].

Using the temperature dependences of the thermal pressure $P(T)$ (Fig. 2) and the isochoric heat conductivity $\lambda_V(T)$ (Fig. 3), we constructed the isothermal dependences $\lambda_T(P)$ of the heat conductivity of solid CO_2 and NH_3 on the pressure that arises in the studied specimens as their molar volume changes. The results are displayed in Fig. 4.

Using the methods of computer simulation, the isothermal heat conductivity λ_T of both CO_2 and NH_3 was revealed to vary, as the pressure grows, according to the dependence

$$\lambda_T = A(T) + B(T)P + C(T)P^2, \quad (3)$$

where A , B , and C are the numerical coefficients, the values of which are listed in Table 1 for various temperatures. With increase in pressure at a constant temperature, the heat conductivity also increases (Fig. 4). Table 1 includes also the variations $\Delta\lambda_T$ of the heat conductivity values, which are governed by the increase of pressure ΔP . For comparison, in the course of studying the dependence of the isothermal heat conductivity of solid C_6H_6 on pressure [24], the increase of pressure by $\Delta P = 600$ MPa at $T = 300$ K resulted in the variation of the heat conductivity $\Delta\lambda_T = 0.33$ W/(m·K). As is seen from Fig. 2, the thermal pressure which arises in the solid CO_2 and NH_3 specimens and the pressure which induces the variation of the isothermal heat conductivity of solid C_6H_6 upon direct experimental researches are close to each other, which indicates the eligibility of the assumption concerning the influence of thermal pressure upon isochoric heat conductivity.

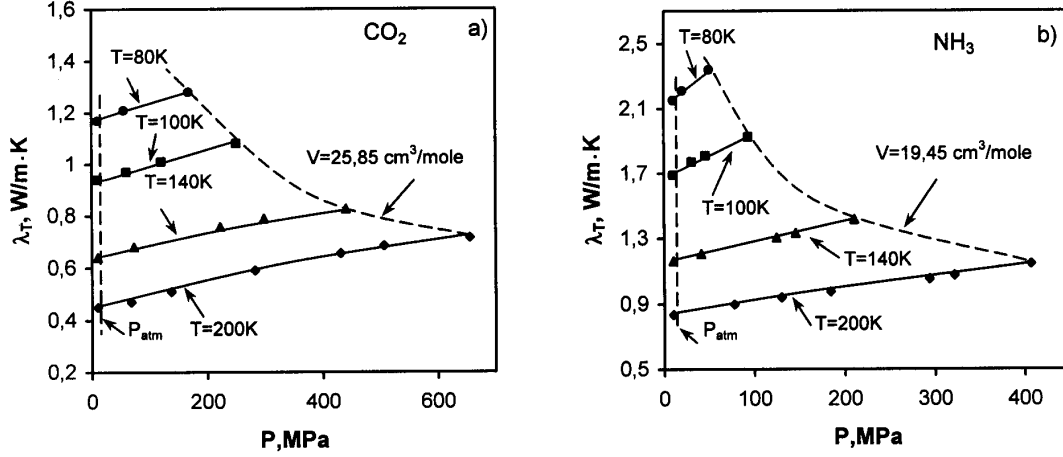


Fig. 4. Isothermal dependences of the heat conductivity of solid CO_2 (a) and NH_3 (b) on the pressure $\lambda_T(P)$. P_{atm} is the value of the heat conductivity that corresponds to atmospheric pressure

The value A^* of the first coefficient in relation (3), normalized to the temperature and the molar volume, is practically constant for various temperatures (see Table 1). The coefficient A in (3) is nothing else but the value of isobaric heat conductivity. The fact that this coefficient, normalized to the temperature and the molar volume, is constant evidences for the additional dependence of isobaric heat conductivity on thermal expansion of the studied specimens. However, the issue of the influence of thermal expansion on the isobaric heat conduction of molecular crystals is not dealt with in this work, so we confine ourselves to a mere statement of this dependence.

Supposing that heat in dielectric crystals is transferred mainly by phonons, we use the following dependence to determine the phonon contribution to the heat conductivity at temperatures of the order of or higher than the Debye one ($T \geq \Theta_D$) [22]:

$$\lambda_{\text{ph}} = K \frac{ma\Theta_D^3}{\gamma^2 T} \quad (4)$$

Here, m is the molecular mass, a^3 is the volume of a single atom (molecule), and K is the structural factor (see Table 2). The results of calculations of the phonon heat conductivity in solid CO_2 and NH_3 for specimens with the molar volumes $V_{\text{mol}} = 25.85$ and $19.45 \text{ cm}^3/\text{mol}$, respectively, are depicted in Fig. 1. The calculations were fulfilled in the framework of relation (4) and gave the classical dependence of the heat conductivity $\lambda_{\text{ph}} \propto T^{-1}$. As is seen from Fig. 1, the values of the isochoric heat conductivity are overestimated as compared to the law $1/T$. Such a behavior of λ_V can be connected to the influence of

thermal pressure that increases in a specimen with the temperature. If the influence of thermal pressure is taken into account, the isochoric heat conductivity can be determined as the sum of the phonon heat conductivity and an additional component governed by the influence of thermal pressure:

$$\lambda_V = \lambda_{\text{ph}} + \Delta\lambda_V, \quad (5)$$

where the quantity $\Delta\lambda_V$ is the additional contribution of thermal pressure to isochoric heat conductivity.

Table 1. Dependences of the heat conductivity $\Delta\lambda_T$, the pressure ΔP , the coefficients A , B , and C of the isothermal dependence $\lambda_T = A(T) + B(T)P + C(T)P^2$, and the coefficient A^* on the temperature for solid CO_2 and NH_3

T , K	A	B	C	A^*	$\Delta\lambda_T$, W/(m·K)	ΔP , MPa
CO_2						
80	1.160	0.0014	$-2 \cdot 10^{-6}$	2435.07	0.11	167.5
100	0.920	0.0009	$-3 \cdot 10^{-7}$	2435.25	0.14	250.1
140	0.644	0.0007	$-6 \cdot 10^{-7}$	2435.22	0.18	440.2
200	0.434	0.0005	$-3 \cdot 10^{-6}$	2434.59	0.26	655.3
NH_3						
80	2.08	0.0066	$-9 \cdot 10^{-8}$	3284.32	0.19	49.7
100	1.651	0.0041	$-3 \cdot 10^{-7}$	3284.49	0.23	93.2
140	1.162	0.0012	$-1 \cdot 10^{-5}$	3284.57	0.25	210.6
190	0.836	0.0008	$-3 \cdot 10^{-5}$	3283.78	0.31	406.8

Table 2. The values of the fitting coefficients K and K_1 and other quantities which were used for the calculation of the isochoric heat conductivity of solid CO_2 and NH_3 specimens with the molar volume $V_{\text{mol}} = 25.85$ and $19.45 \text{ cm}^3/\text{mol}$, respectively

Substance	v , m/s	a , 10^{-10} m	γ	g	ΔT , K	K , 10^{-4} s/K	K_1 , 10^{-3} s/K
CO_2	1821.3	3.58	2.5	5.7	167.5	1.43	3.26
NH_3	2629.6	3.25	1.2	5.2	142.6	2.11	2.88

The heat conductivity $\Delta\lambda_V$ results from the influence of thermal pressure and must depend functionally on this parameter. Making use of formula (1), we obtain

$$\Delta\lambda_V = K_1 \frac{\gamma C_V \Delta T}{V_{\text{mol}}}, \quad (6)$$

where K_1 is the fitting parameter and $\Delta T = T - T_{V=\text{const}}$ defines the temperature interval where the isochoric condition holds true.

Substituting relations (4) and (6) into (5), the isochoric heat conductivity can be written down as

$$\lambda_V = K \frac{ma \Theta_D^3}{\gamma^2 T} + K_1 \frac{\gamma C_V \Delta T}{V_{\text{mol}}}. \quad (7)$$

Matching the units of the K and K_1 coefficients with those of the heat conductivity, formula (7) reads

$$\lambda_V = K \left(\frac{k_B}{\hbar} \right) \frac{ma \Theta_D^3}{\gamma^2 T} + K_1^2 \left(v^2 \frac{\hbar}{k_B} \right) \frac{\gamma C_V \Delta T}{V_{\text{mol}}}, \quad (8)$$

where k_B is the Boltzmann constant, \hbar is the Planck's constant divided by 2π , K and K_1 are the fitting coefficients, the values of which are quoted in table 2, and v is the average sound velocity that was calculated according to the data of work [26].

As the temperature grows, the additional heat conductivity $\Delta\lambda_V$ caused by thermal pressure (Fig. 1) increases and becomes larger than the error of experiment (5%) at temperatures close to 70 and 110 K for solid CO_2 and NH_3 , respectively. That is, we may say that those temperatures define the threshold values of thermal pressure, above which one may talk about an essential influence of thermal pressure on isochoric heat conductivity. For the specimens of solid CO_2 and NH_3 with the molar volumes $V_{\text{mol}} = 25.85$ and $19.45 \text{ cm}^3/\text{mol}$, respectively, the relevant threshold values are $P_{\text{thresh}} = 128.1$ and 119.8 MPa (see Fig. 2).

The curves calculated according to formula (8) (see the solid curves 1 in Fig. 1) describe well the behavior of the isochoric heat conductivity of solid CO_2 and NH_3 . Revealing more general regularities in the behavior of the isochoric heat conductivity of molecular crystals at temperatures of the order of and higher than the Debye temperature requires additional researches of the influence of thermal pressure upon the isochoric heat conductivity of crystals of various symmetry and with various types of thermal motion of molecules.

3. Conclusions

It has been shown in this work that the temperature dependence of the isochoric heat conductivity can be

described by the model where heat conduction is governed by the phonon-phonon interaction and the additional contribution of thermal pressure, with solid CO_2 and NH_3 taken as examples. The obtained dependences $\lambda_T(P)$, $\Delta\lambda_V(T)$, and $P(T)$ made it possible to determine the threshold values of thermal pressure, above which one may talk about a substantial influence of thermal pressure on the isochoric heat conductivity in solid CO_2 ($P_{\text{thresh}} \approx 130 \text{ MPa}$) and NH_3 ($P_{\text{thresh}} \approx 120 \text{ MPa}$), and to reveal the form of the functional dependences of the isochoric heat conductivity that account for the influence of thermal pressure. It should be noted that the presented model can be applied to the calculation of the isochoric heat conductivity values only in the orientationally ordered phases of molecular crystals, since the heat conduction in the orientationally disordered phases of molecular crystals depends essentially on the character of the orientational motion of molecules as well [21,25]. The issue concerning the influence of phase transitions on the isochoric heat conductivity is also of interest because, as is well-known [26], owing to the thermal pressure occurring in isochoric experiments, the temperatures of phase transitions T_m shift towards higher values, which can affect the translational heat conduction.

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КОРЕЛЯЦІЯ МІЖ ТЕРМІЧНИМ ТИСКОМ І ІЗОХОРНОЮ ТЕПЛОПРОВІДНІСТЮ У ТВЕРДИХ CO₂ І NH₃

О.І. Пурський, В.С. Ковтуненко

Резюме

Проведено аналіз взаємозв'язку між термічним тиском та ізохорною теплопровідністю у твердих CO₂ і NH₃. Отримано температурні залежності термічного тиску й ізохорної теплопровідності для зразків з різними молярними об'ємами. Проведено розрахунок ізотермічних залежностей теплопровідності твердих CO₂ і NH₃ від тиску. Встановлено вигляд температурної залежності ізохорної теплопровідності з урахуванням термічного тиску. Характер температурної залежності ізохорної теплопровідності твердих CO₂ і NH₃ визначається фонон-фононою взаємодією та додатковим впливом термічного тиску.