

The lower limit of thermal conductivity in multicomponent solutions of rare gas solids

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Received October 24, 2018

The isochoric thermal conductivity of $\text{Kr}_{0.63}\text{Xe}_{0.37}$ solid solution has been investigated for three samples with different molar volumes in the temperature range from 80 K to the onset of melting, as well as the thermal conductivity of the ternary ($\text{Kr}_{0.63}\text{Ar}_{0.185}\text{Xe}_{0.185}$) and quaternary ($\text{Kr}_{0.63}\text{Ar}_{0.12}\text{Xe}_{0.12}(\text{CH}_4)_{0.13}$) solid solutions. It is found that for multi-component alloys, the thermal conductivity reaches a minimum, whereby adding more impurity atoms in the solid solution does not affect the thermal conductivity in agreement with the recent nonequilibrium molecular dynamics calculations for argon. The phonon contribution to the total thermal conductivity depends significantly on molar volume of sample and impurity concentration, in contrast to the contribution of diffusive modes, which is practically independent of these factors.

Keywords: thermal conductivity, rare gas solids, solid solutions, phonon, diffuson.

Introduction

Rare gas solids (RGS) Ar, Kr and Xe refer to the simplest substances whose atoms are connected by a weak van der Waals interaction and interatomic potential can be relatively easily modeled. They form crystals with *fcc* structure and do not have phase transitions up to the melting point. As a consequence the RGS are ideal objects for comparing experimental data with theory. A large number of experimental [1–9] and theoretical [10–19] studies have been devoted to examination of their thermal conductivity. Initially, a theoretical analysis of the thermal conductivity of dielectric crystals was carried out using the Boltzmann transport equation for phonons [20]. It is assumed that in a perfect crystal at temperatures of the order and above corresponding Debye temperature ($T \geq \Theta_D$) the main mechanism determining magnitude and temperature dependence of the thermal conductivity $\kappa(T)$ is phonon–phonon interaction. Above Θ_D the lifetime of three-phonon scattering processes is inversely proportional to temperature while the specific heat and phonon group velocity are considered as temperature independent. In combination with the kinetic theory of phonon gas, this leads to the well-known $\kappa \propto T^{-1}$ dependence of the thermal conductivity of dielectric solids [20]. In practice the T^{-1} dependence is actually observed at some fraction of the Debye temperature, for example at $\Theta_D/4$ for argon and at $\Theta_D/10$ for silicon.

More sharp decrease of thermal conductivity with increasing temperature observed in the heavy RGS at a saturated vapor pressure was initially erroneously attributed to higher-order four-phonon interactions [3]. It was later shown experimentally [7–9] that such behavior is related to the thermal expansion of the crystal (the molar volumes of RGS changes on the order of 10% in temperature interval from 0 K to the melting point), and the isochoric thermal conductivity can be described as the sum of two contributions: from propagating phonons and localized "diffuse" modes: $\kappa = \kappa_{\text{ph}} + \kappa_{\text{dif}}$ or

$$\kappa = A/T + B, \quad (1)$$

where the coefficients A and B do not depend on temperature. Afterwards, the isochoric thermal conductivity of RGS and a number of molecular crystals was described in the framework of standard Debye expression for thermal conductivity [20] under the assumption that the mean-free path of a phonon cannot become less than half of its wavelength or lattice constant. This idea was first proposed by Roufosse and Klemens [21]. Accounting for this circumstance leads to the fact that the thermal conductivity is described, respectively, by the expressions $\kappa = A/T^2 + B$ and $\kappa = A/T^{3/2} + B$ [22,23]. In both cases, the phonon contribution to the thermal conductivity decreases steeper than in the case of $1/T$ dependence, because the borderline between high-frequency "diffusive" modes and low-frequen-

cy phonons is shifted downward with increasing temperature and, consequently, the number of phonon modes decreases.

While simple Debye model of thermal conductivity does yield useful insight, it has substantial limitations. The weakness of this approach is that it assumes a linear dispersion law up to the end of Brillouin zone and a quadratic density of phonon states thereby it completely ignores the real dispersion of phonons and the real density of their states. The assumption that a solid has the Debye dispersion leads to the contribution of high frequency phonons being substantially overvalued because actual zone-edge phonons have a much smaller group velocity than the sound velocity. Attempts to artificially incorporate the dispersion into consideration using fitting parameters do not lead to satisfactory results [24].

In recent years *ab initio* calculations of the thermal properties of disordered systems based on the Green Cubo approach using molecular (MMD) or lattice dynamics methods have developed extensively [25–27]. This method makes it possible to calculate as well the thermal conductivity of ordered solids, in particular, the thermal conductivity of crystalline argon [14–19]. Using MMD and the *Green–Kubo* method, it was shown that the thermal conductivity of a Lennard-Jones *fcc* crystal of argon is described by two time constants associated with the attenuation of the autocorrelation function of the heat flow. The first time scale is associated with short-wave phonons, which have an average mean-free path equal to half the wavelength, and corresponding contribution to the thermal conductivity does not depend on temperature. The second time scale is longer and corresponds to acoustic phonons with a mean-free path greater than half their wavelength, and corresponding contribution to the thermal conductivity decreases with increasing temperature. Advances in the measurement and computation of thermal phonon transport properties are detailed for example in [27].

Despite the abundance of information, it can be argued that the dependence of the isochoric thermal conductivity of Ar, Kr and Xe on temperature and molar volume has not

been strictly established by experiment. It was assumed initially that the coefficients A and B depend in the same way on the molar volume $\kappa = (A/T+B)(V_0/V)^g$, where V_0 is molar volume at 0 K, V is molar volume of a sample, and $g = -(\partial \ln \kappa / \partial \ln V)_T$ is the Bridgman coefficient [9]. In the later it was shown that this is not true [23]. To clarify the temperature dependence of the isochoric thermal conductivity of RGS experimental data for of Ar, Kr and Xe were represented in the reduced coordinates $\kappa T(T)$, $\kappa T^{3/2}(T^{3/2})$ и $\kappa T^2(T^2)$ (see Figs. 1–3). In all mentioned above coordinates, when the corresponding dependence is fulfilled, the experimental points must lie on a straight line. An unambiguous conclusion about the degree of dependence of thermal conductivity on temperature is difficult to make on the basis of the graphs. It is only possible to affirm that the isochoric thermal conductivity is described with good accuracy by the expression $\kappa = AT^n+B$, where n varies between 1 and 2 with the appropriate choice of coefficients A and B . The dependence $\kappa = A/T+B$ is well satisfied for krypton and xenon, and for argon it is valid only above 90 K. This may be due to the fact that the Debye temperature of argon (93.3 K) is higher than its triple point (83.8 K). In the future we will use this dependence because it proceeds from more accurate physical representations and is confirmed by direct *ab initio* calculations. It was shown recently that the interface between fast acoustic phonons with the dispersion law close to the sound (propagons) and phonons, which propagate much slower (diffusons), whose dispersion law is different from the sound one, coincides with the first van Hove singularity [28,29].

Point defects cause additional scattering of phonons and, consequently, a decrease in thermal conductivity. At low concentrations, the point defects give a small constant additive to the thermal resistance $W = 1/\kappa$ at high temperatures. In the case of strong scattering, the thermal conductivity is usually weakly dependent on the impurity concentration. The isochoric thermal conductivity of solid krypton with methane and xenon admixtures was studied in the temperature range $T \geq \Theta_D$ in number of studies [22,30–34], there are also examples of *ab initio* calculations of the ther-

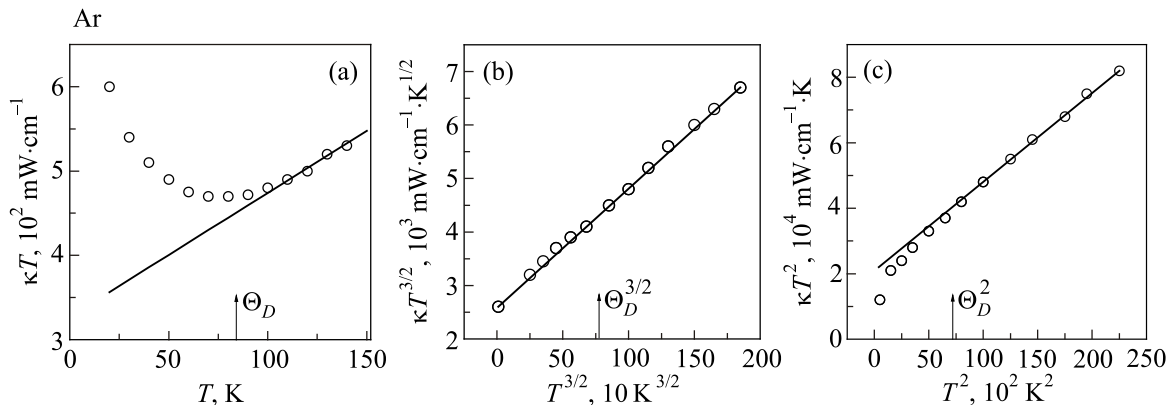


Fig. 1. Isochoric thermal conductivity of Ar ($V_m = 22.14 \text{ cm}^3/\text{mole}$) [7] represented in coordinates: $\kappa T(T)$ (a), $\kappa T^{3/2}(T^{3/2})$ (b), $\kappa T^2(T^2)$ (c).

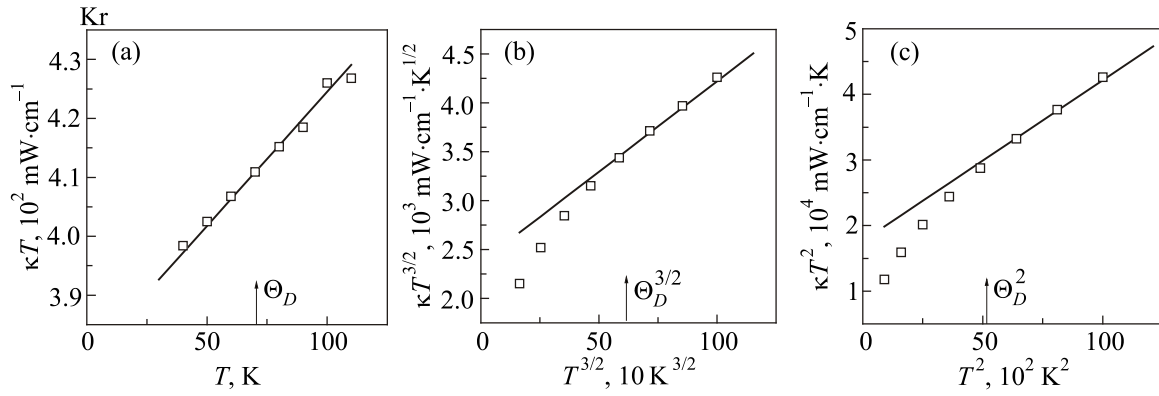


Fig. 2. Isochoric thermal conductivity of Kr ($V_m = 27.1 \text{ cm}^3/\text{mole}$) [8,9] represented in coordinates: $\kappa T(T)$ (a), $\kappa T^{3/2}(T^{3/2})$ (b), $\kappa T^2(T^2)$ (c).

mal conductivity of solid argon with impurities [35–37]. The Kr–CH₄ system demonstrates the complete solubility of the components, the same occurs in the Kr–Xe system above 75 K [38]. It was found that as the impurity concentration increases, the phonon contribution to thermal conductivity decreases, and the thermal conductivity itself approaches its lower limit as it was interpreted by Cahill, Watson and Pohl [39]:

$$\kappa_{\min} = \frac{1}{2} \left(\frac{\pi}{6} \right)^{1/3} k_B n^{2/3} (v_l + 2v_t), \quad (2)$$

where v_l and v_t are the longitudinal and transverse sound velocities, n is the number of atoms (molecules) per unit volume. With an increase in the impurity concentration above 10%, the thermal conductivity remained almost unchanged [22,32]. It was also found that as the part of heat carried by the “diffuse” modes increased, the Bridgman coefficient $g = -(\partial \ln \kappa / \partial \ln V)_T$ decreased from the value $g \approx 9\text{--}10$, which is characteristic for pure crystals up to $g \approx 3\text{--}4$, more typical for glasses and amorphous solids.

Expression (2) is essentially a modification of the Einstein model of thermal conductivity in which atoms in a crystal lattice perform harmonic oscillations of the same frequency and are connected by harmonic forces. In order to eliminate the uncertainty in the choice of the Einstein

frequency, Cahill, Watson, and Pohl [39] modified the theory by including vibrations with a larger length. Thermal conductivity is determined by random walk of thermal energy between neighboring localized quantum mechanical oscillators, the lifetime of each of which was assumed to be equal to half the oscillation period. It is clear that such a description sins with all the deficiencies inherent in the primitive Debye model, primarily due to ignoring the real dispersion law and density of states of phonons, and we can talk only about how justified its use for the evaluation of the lower limit of the thermal conductivity.

The revival of interest in the systems mentioned above is connected with the need to systematize and re-evaluate the experimental results on the basis of a more realistic model and to refine the volume dependence of the coefficients A and B in the expression (1) for the thermal conductivity. It was also stimulated by the theoretical calculations [37], where the effect of mass disorder on the thermal conductivity of alloys with four or more components was evaluated. To predict the thermal conductivity of solid solutions, modeling using the nonequilibrium molecular dynamics (NEMD) method was performed using the Lennard-Jones potential (LJ) and one to five atomic components. It was shown that for multicomponent solutions, the thermal conductivity reaches a minimum, as a

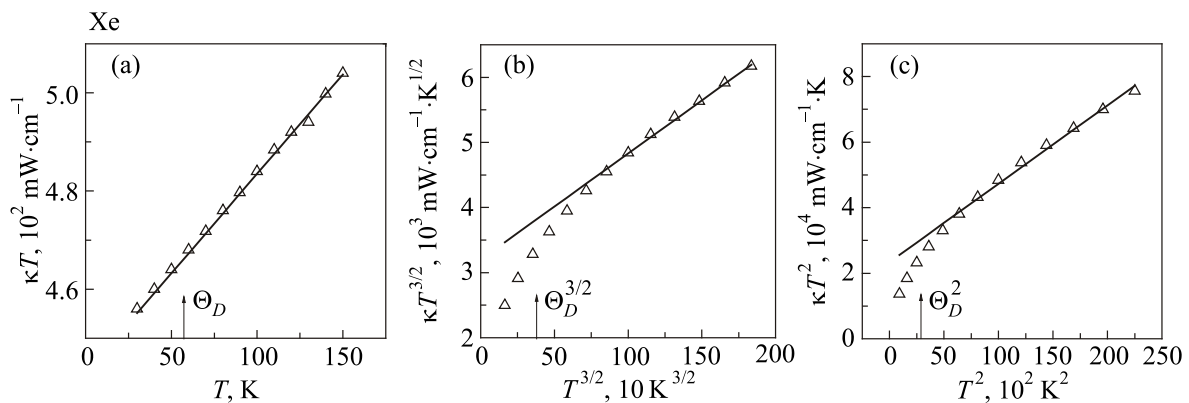


Fig. 3. Isochoric thermal conductivity of Xe ($V_m = 34.6 \text{ cm}^3/\text{mole}$) [9] represented in coordinates: $\kappa T(T)$ (a), $\kappa T^{3/2}(T^{3/2})$ (b), $\kappa T^2(T^2)$ (c).

result of which the addition of impurities to it does not affect the thermal conductivity. NEMD calculations show that to further reduce the thermal conductivity of multi-component solutions, local deformation fields must be perturbed by a change in the interatomic force field. In addition it was shown that with additional scattering due to changes in the local force field (i.e., phonon scattering due to changes in the bond and / or volume) the NEMD predicts that the thermal conductivity of the crystalline alloy may be lower than in the amorphous phase. This suggests that for solid solutions with five or more kinds of atoms the inclusion of local strain-field for additional phonon scattering can lead to an isotropic crystalline material with ultra-low thermal conductivity that can be lower than the predicted minimum limit for the corresponding amorphous phases. All of the above prompted us to study the thermal conductivity of the three-component Kr, Ar and Xe and four-component Kr, Ar, Xe, and CH₄ solid solutions.

Experimental results and their discussion

Studies at a constant volume can be realized for molecular solids having relatively high compressibility and large coefficients of thermal expansion. If a solid sample of a sufficiently high density is grown in a high-pressure cell, it can subsequently be cooled at a practically constant volume, while the pressure in the cell decreases. Usually, it falls to zero at some characteristic temperature T_0 , below which the condition of constancy of the density is violated. Further cooling of the sample may be accompanied by its cracking and detachment from the cell walls. At constant density melting of the sample occurs in a certain temperature interval and its beginning shifts toward high temperatures. According to the melting curves of RGS [40] this shift may be of 40–50 K at a pressure of 100 MPa in the cell.

The present studies were carried out by the steady-state heat flux method in a cell of coaxial geometry [41]. The samples were grown at pressures from 30 to 100 MPa, produced using an auxiliary thermo compressor, with the temperature gradient along the cell being about 1.5 K/cm. After growing of the sample the inlet capillary was blocked by freezing with liquid nitrogen, and the sample was annealed at a temperature of 100 K for 4–5 hours. At the end of measurements the sample was re-condensed into a thin-walled vessel and its mass was determined by weighing. The molar volume of the sample was calculated from the known volume of the measuring cell and the mass of the sample. The systematic measurement error was $\pm 4\%$.

The isochoric thermal conductivity of Kr_{0.63}Xe_{0.37} solid solution was investigated for three samples with molar volumes V_m of 32.0, 31.5 and 31.2 cm³/mole (denoted as Nos. 1–3, respectively) in the temperature range from 80 K to the onset of melting (see Fig. 4). Figure 5 shows isochoric thermal conductivity of pure Kr ($V_m = 28.5$ cm³/mole, asterisks), solid Kr_{0.63}Xe_{0.37} solution ($V_m = 31.2$ cm³/mole, No. 3, asterisks), solid Kr_{0.63}Xe_{0.37} solution ($V_m = 31.2$ cm³/mole, Nos. 1–3, respectively) in the temperature range from 80 K to the onset of melting (see Fig. 4). Figure 5 shows isochoric thermal conductivity of pure Kr ($V_m = 28.5$ cm³/mole, asterisks), solid Kr_{0.63}Xe_{0.37} solution ($V_m = 31.2$ cm³/mole, No. 3, asterisks), triple Kr_{0.63}Ar_{0.185}Xe_{0.185} (No. 4, triangles) and quadruple Kr_{0.63}Ar_{0.12}Xe_{0.12}(CH₄)_{0.13} (No. 5, squares) solid solutions. A closer view of the thermal conductivity of solid solutions is shown in the inset.

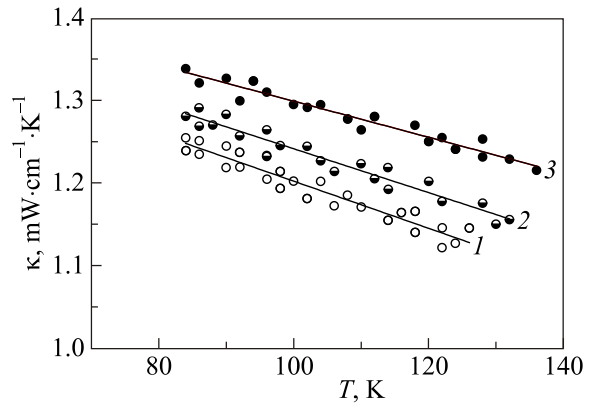


Fig. 4. Isochoric thermal conductivity of solid Kr_{0.63}Xe_{0.37} solution for three samples with different molar volumes (V_m) of 32.0, 31.5 and 31.2 cm³/mole, (denoted as Nos. 1–3, respectively).

No. 3), as well as triple Kr_{0.63}Ar_{0.185}Xe_{0.185} (No. 4, triangles) and quadruple Kr_{0.63}Ar_{0.12}Xe_{0.12}(CH₄)_{0.13} (No. 5, squares) solid solutions. A closer view of the thermal conductivity of solid solutions is shown in the inset. Samples No. 1 and No. 2 were grown at pressures of 30 and 60 MPa, respectively, samples No. 3, 4, and 5 were grown at pressures of 90 MPa. The smoothed values of the isochoric thermal conductivity are shown by solid lines. The concentration of solutions is indicated for the gas phase.

Information on the phase diagram of the ternary and quaternary solutions is absent, but separately all components are unrestrictedly dissolved in Kr at pre-melting temperatures [38]. The Bridgman coefficient, calculated from our experimental data for Kr_{0.63}Xe_{0.37} solution, is 3.7 ± 1.5 at 100 K, which is close to 4.0 ± 1.5 for a solid solution Kr_{0.86}Xe_{0.14} [32]. For reference the lower limit of the

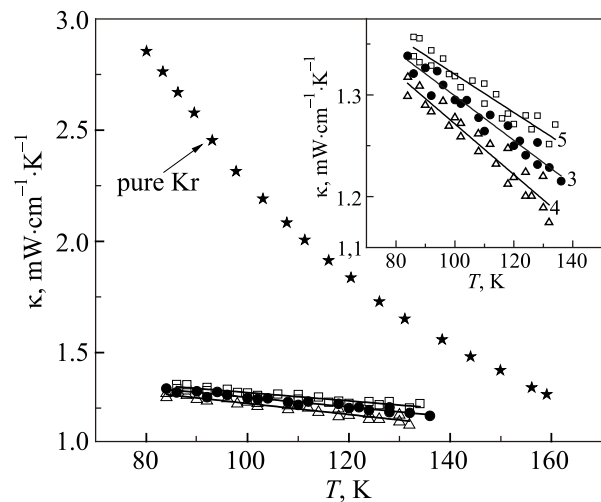


Fig. 5. Isochoric thermal conductivity of pure Kr ($V_m = 28.5$ cm³/mole, asterisks), solid Kr_{0.63}Xe_{0.37} solution ($V_m = 31.2$ cm³/mole, No. 3, asterisks), triple Kr_{0.63}Ar_{0.185}Xe_{0.185} (No. 4, triangles) and quadruple Kr_{0.63}Ar_{0.12}Xe_{0.12}(CH₄)_{0.13} (No. 5, squares) solid solutions. A closer view of the thermal conductivity of solid solutions is shown in the inset.

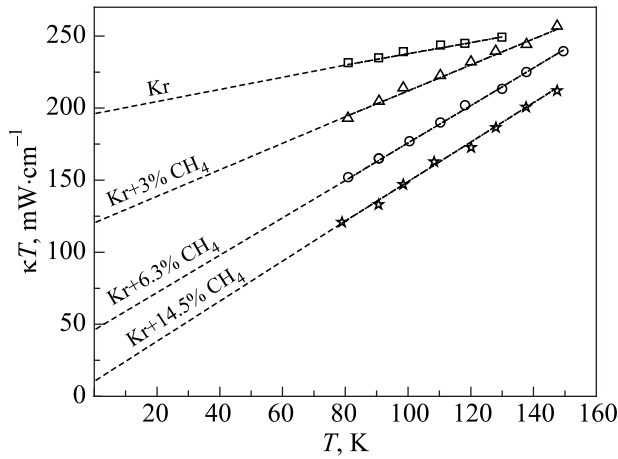


Fig. 6. Isochoric thermal conductivity of Kr with CH₄ admixture represented in coordinates $\kappa T(T)$.

thermal conductivity κ_{\min} of Kr, calculated according to the Eq. 2 using data of [40] is $1.1 \text{ mW}\cdot\text{cm}^{-1}\cdot\text{K}^{-1}$ [22]. Direct calculations of the lower limit of thermal conductivity by the NEMD method for Kr were not carried out, however, it can be estimated from calculations for LJ Ar using the method of reduced coordinates [3]. According to the estimates, its value is $1.4 \text{ mW}\cdot\text{cm}^{-1}\cdot\text{K}^{-1}$, which is somewhat higher than the value obtained from Eq. (2).

It is seen that the thermal conductivities of double, triple and quaternary solid solutions are close to each other and to the calculated lower limit of thermal conductivity κ_{\min} . The isochoric thermal conductivity near its lower limit weakly depends on temperature, molar volume of the solutions, concentration of the components, and addition of new ones, as predicted by NEMD calculations using the LJ potential for argon [37]. To determine the dependence of the coefficients A and B on the molar volume, the experimental results for the solution $\text{Kr}_{0.63}\text{Xe}_{0.37}$ were presented in coordinates $\kappa T(T)$. All of them fit well into straight lines, and the coefficients were determined by extrapolation. The partial Bridgman coefficient $g_A = -(\partial \ln A / \partial \ln V)_T$ is 13 ± 1.5 .

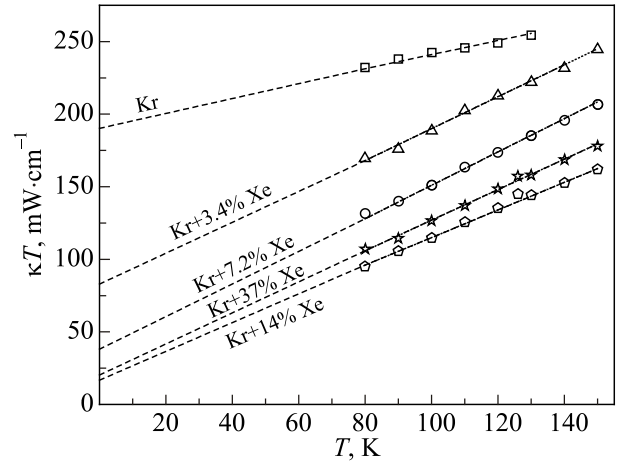


Fig. 7. Isochoric thermal conductivity of Kr with Xe admixture represented in coordinates $\kappa T(T)$.

The total Bridgman coefficient is averaged over phonons and diffusive modes [23]

$$g = \frac{\kappa_{\text{ph}}}{\kappa} g_A + \frac{\kappa_{\text{dif}}}{\kappa} g_B. \quad (3)$$

Due to the weak dependence of the parameter B on the density, the Bridgman coefficient $g_B = -(\partial \ln B / \partial \ln V)_T$ is determined from the slope of the lines in the coordinates $\kappa T(T)$ with a large error. Therefore, we calculated it from the already known coefficients g and g_A and relation (3). It is equal to $g_B = 2 \pm 1.5$. According to the data of [22,32], the Bridgman coefficient $g = -(\partial \ln \kappa / \partial \ln V)_T$ decreases from $g \approx 9-10$, characteristic for pure Kr, to $g \approx 3-4$ with an increase in the impurity concentration of Xe or CH₄ to 10%.

The experimental data [22,32] for different concentrations of Xe and CH₄ are presented in Figs. 6 and 7 in coordinates $\kappa T(T)$. Information about the impurity concentration, molar volumes of samples V_m , coefficients A , B and the Bridgman coefficients $g = -(\partial \ln \kappa / \partial \ln V)_T$ are also shown in Table 1. It can be seen that for the $\text{Kr}_{0.63}\text{Xe}_{0.37}$ samples with different molar volumes, the coefficient A

Table 1. Impurity concentration, molar volumes V_m of samples, fitting coefficients A and B , Bridgman coefficients $g = -(\partial \ln \kappa / \partial \ln V)_T$

Solution	$V_m, \text{cm}^3/\text{mole}$	$A, \text{mW}/\text{cm}$	$B, \text{mW}/(\text{cm}\cdot\text{K})$	g
pure Kr	28.5	195	0.45	9.4 ± 1.5
$\text{Kr}_{0.97}(\text{CH}_4)_{0.03}$	28.6	120	0.95	8.5 ± 1.5
$\text{Kr}_{0.937}(\text{CH}_4)_{0.063}$	28.8	44	1.1	7.7 ± 1.5
$\text{Kr}_{0.855}(\text{CH}_4)_{0.145}$	29.25	16	1.2	5.2 ± 1.5
$\text{Kr}_{0.966}\text{Xe}_{0.034}$	29.0	80	1.05	8.0 ± 1.5
$\text{Kr}_{0.928}\text{Xe}_{0.072}$	29.5	43	1.1	5.5 ± 1.5
$\text{Kr}_{0.86}\text{Xe}_{0.14}$	30.0	17	1.0	4.0 ± 1.5
$\text{Kr}_{0.63}\text{Xe}_{0.37}$	32.0	22	1.0	3.7 ± 1.5
$\text{Kr}_{0.63}\text{Xe}_{0.37}$	31.5	27	1.0	
$\text{Kr}_{0.63}\text{Xe}_{0.37}$	31.2	30	1.0	
$\text{Kr}_{0.63}\text{Ar}_{0.185}\text{Xe}_{0.185}$	–	29	1.0	–
$\text{Kr}_{0.63}\text{Ar}_{0.12}\text{Xe}_{0.12}(\text{CH}_4)_{0.13}$	–	32	1.0	–

responsible for the phonon contribution depends significantly on the density (molar volume), while B describing the diffuse contribution is practically constant. The same applies to concentration dependence. Coefficient A changes practically by an order of magnitude from pure Kr to solid solutions with a maximum concentration of impurities, while B is practically the same except for pure Kr where it is twice lower. Estimates of the partial Bridgman coefficients from the data of [22,32] for different concentrations of Xe and CH₄ in Kr vary within $g_A = 12\text{--}18$ and $g_B = 1\text{--}4$. Theoretical estimates give $g_A = 3\gamma + 2q - 1/3$ for phonon modes and $g_B = \gamma + 1/3$ for “diffusive” modes [23,33,42], where γ is the Grüneisen parameter and $q = (\partial \ln \gamma / \partial \ln V)_T \approx 1$ [42,43]. Taking the value of $\gamma = 2.85$ for Kr [40], we have $g_A = 10.3$ and $g_B = 2.5$, which is in reasonable agreement with the experiment.

Conclusions

The isochoric thermal conductivity of Kr_{0.63}Xe_{0.37} solid solution has been investigated for three samples with different molar volumes in the temperature range from 80 K to the onset of melting, as well as the thermal conductivity of the ternary (Kr_{0.63}Ar_{0.185}Xe_{0.185}) and quaternary (Kr_{0.63}Ar_{0.12}Xe_{0.12}(CH₄)_{0.13}) solid solutions. The thermal conductivities of double, triple and quaternary solid solutions are close to each other and to the calculated lower limit of thermal conductivity κ_{\min} . The thermal conductivity weakly depends on temperature, density, component concentration and addition of new ones, as predicted by NEMD calculations using the Lennard–Jones potential for argon. Addition of a methane impurity to the ternary Ar/Kr/Xe solution did not lead to a decrease in the thermal conductivity below κ_{\min} . It is shown that coefficient A responsible for the phonon contribution depends essentially on the density (molar volume) and the impurity concentration, while the coefficient B describing the diffuse contribution is practically constant. The Bridgman coefficient $g = -(\partial \ln \kappa / \partial \ln V)_T$ decreases from $g \approx 9\text{--}10$, characteristic for pure Kr, to $g \approx 3\text{--}4$ with an increase in the concentration of Xe and CH₄ impurities above 10%. The partial Bridgman coefficients for different concentrations of Xe and CH₄ in Kr vary within $g_A = 12\text{--}18$ and $g_B = 1\text{--}4$, which agrees reasonably with the theoretical estimates $g_A = 10.3$ and $g_B = 2.5$.

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Нижня межа теплопровідності
мультikomпонентних розчинів затверділих
інертних газів

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Досліджено ізохорну теплопровідність твердого розчину $Kr_{0,63}Xe_{0,37}$ для трьох зразків з різними молярними об'ємами в інтервалі температур від 80 К до початку плавлення, а та-

кож теплопровідність потрійного ($Kr_{0,63}Ar_{0,185}Xe_{0,185}$) та чотирьохкомпонентного ($Kr_{0,63}Ar_{0,12}Xe_{0,12}(CH_4)_{0,13}$) твердих розчинів. Виявлено, що для багатоконпонентних розчинів теплопровідність досягає мінімуму, в результаті чого подальше додавання домішкових атомів в твердий розчин не впливає на теплопровідність відповідно до недавніх розрахунків з використанням методів нерівноважної молекулярної динаміки (NEMD) для аргону. Фононний внесок в теплопровідність істотно залежить від молярного об'єму зразка та концентрації домішки, на відміну від вкладу дифузних мод, який практично не залежить від цих чинників.

Ключові слова: теплопровідність, затверділі інертні гази, тверді розчини, фонон, дифузон.

Нижний предел теплопроводности
мультikomпонентных растворов отвердевших
инертных газов

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Исследована изохорная теплопроводность твердого раствора $Kr_{0,63}Xe_{0,37}$ для трех образцов с разными молярными объемами в интервале температур от 80 К до начала плавления, а также теплопроводность тройного ($Kr_{0,63}Ar_{0,185}Xe_{0,185}$) и четырехкомпонентного ($Kr_{0,63}Ar_{0,12}Xe_{0,12}(CH_4)_{0,13}$) твердых растворов. Обнаружено, что для многокомпонентных растворов теплопроводность достигает минимума, в результате чего дальнейшее добавление примесных атомов в твердый раствор не влияет на теплопроводность в соответствии с недавними расчетами с использованием методов неравновесной молекулярной динамики (NEMD) для аргона. Фононный вклад в теплопроводность существенно зависит от молярного объема образца и концентрации примеси, в отличие от вклада диффузных мод, который практически не зависит от этих факторов.

Ключевые слова: теплопроводность, отвердевшие инертные газы, твердые растворы, фонон, дифузон.