Relation between defects and crystalline thermal conduction

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Abstract Modeling of the heat transfer in ideal crystal lattice with defects is performed for measuring the heat conductivity coefficient. A non-steady process in closed system is studied. The method is based on comparison of the results of molecular dynamics simulation and solution of the the heat equation. Two-dimensional and three-dimensional structures with dense packing of particles are considered. Defects are modeled by removing or changing the mass of randomly selected lattice atoms. Based on the results of molecular-dynamics modeling, an empirical dependence of the thermal diffusivity on the density of defects is elaborated. It also turns out in a good agreement with experimental data.

Introduction

Establishing a link between microscopic and macroscopic description of solids requires an understanding of heat transfer at microlevel [1,2]. An interest in the study of an influence of the lattice defects on the heat conductivity has arisen recently due to rapid development in the last decades of the modeling methods based on the molecular dynamics technique. These methods allowed to realize previously developed theoretical approaches [3–5]. The approaches used various simplifications of the phonon Boltzman equation or employ the perturbation theory to describe lattice imperfections. Only a few theoretical papers do not utilize the molecular dynamics methods, see, e.g., [6]. The heat trnasfer in lattice models have been mainly addressed in the context of the steady-state heat conduction [7–10]. Recent works more focus on unsteady conduction regimes [11–18].

The molecular dynamics studies of the heat conductivity variations in the presence of defects cover wide class of materilas. In particular, graphene thermal

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properties have been investigated in [19–24]. The effect of defects and various modifications of atoms on its thermal properties was considered in [20, 22, 24]. Thermal conductivity of flakes of finite-sized doped graphene with an emphasis on the influence of the mass of the substitutional atoms were studied in [19]. In Ref. [21] the influence of the defects position on the thermal conductivity was considered for single-layer graphene nanoribbons. The study is conducted using molecular dynamics modeling and theoretical analysis based on the Boltzmann equation. Thermal conductivity of defective Graphene oxide has been studied in [23]. Other materials were also investigated. Using non-equilibrium molecular dynamics simulation, the effect of crystal lattice defects and mechanical deformation on the thermal conductivity in $\mathrm{Mo\,S_2}$ was studied in Ref. [25]. Some nuclear fuels were considered, thorium dioxide in Ref. [26], and actinide oxides in [27].

In all these papers a decrease in the thermal conductivity has been obtained as soon as the concentration of defects increases, and the effect of vacancies is more pronounced than that of substitutions. These predictions have been confirmed in experiments on the defects in diamond [28–31]. However, no analytical dependence of the heat conductivity variations fitting in the numerical results were obtained.

In paper [11] an approach was proposed to measure thermal conductivity in prefect crystal lattices and lattices with vacancies. The approach uses comparison of the results of molecular dynamics simulation and solution of the heat equation. The method considers non-steady process in closed systems, which allows to study the heat processes without influence of the external heat sources such as thermostats [32]. In this paper, the approach is extended to study thermal conductivity in crystal lattices with defects in a form of mass inclusions, which is handy to study practically important problem of the influence of the isotope composition on the heat conduction in crystals. Vacancy-based defects are also considered. Two-dimensional and three-dimensional structures with dense packing of particles are modeled. Empirical dependence of the thermal diffusivity on the density of defects is obtained in an explicit form. It is shown that the obtained dependence describes well the data obtained from the nature experiments with diamonds possessing various isotope composition.

1 Research method

Consider the classical heat equation,

$$\dot{T} - \beta T'' = 0, \tag{1}$$

where β is the thermal diffusivity constant. Let the initial temperature distribution be

$$T|_{t=0} = T_1 + T_2 \sin kx, \quad k = 2\pi/L, \tag{2}$$

where T_1 is the average temperature, T_2 is the amplitude of the temperature deviations, and L is the spatial period of the temperature deviations. It is easy to show that an exact solution with a period L for an equation (1) with initial conditions (2) and periodic boundary conditions is

$$T = T_1 + T_2\, e^{-\beta k^2 t}\, \sin k\, x. \tag{3}$$

Direct measurement of the temperature form the molecular dynamics experiments faces with the problems caused by the random motion deviations. Better precision can be obtained with the use the integral characteristics, which average the deviations. Consider the integral

$$J(t) = \int_0^L \left(T(x,t) - T_1 \right)^2 dx. \tag{4}$$

This integral can be easily calculated in computer experiments. On the other hand, analytic calculation of the integral (4) with solution (3) results in

$$J(t) = \frac{T_2^2 L}{2} e^{-2\beta k^2 t}. \tag{5}$$

This equation allows us to express β through two known values of the integral J at times t_1 and t_2,

$$\beta = \frac{L^2}{8\pi^2 (t_2 - t_1)} \ln \frac{J(t_1)}{J(t_2)}. \tag{6}$$

The thermal conductivity coefficient κ and the thermal diffusivity coefficient β can be obtained from the following system of equations

$$\dot{U} = -q', \qquad \dot{q} = -\kappa T', \qquad \dot{U} = c\dot{T}, \tag{7}$$

where U is the thermal energy per unit volume of the material; q is the heat flux (thermal energy passing per unit of time through a unit of area); c is the heat capacity of a unit volume of material. The first of the equations (7) is the heat energy balance equation, the second is the Fourier thermal conductivity law, the third expresses the relationship between changes in thermal energy and temperature (changes in thermal energy associated with variations in pressure and density are not taken into account). The elimination of U and q from system (7) gives thermal conductivity equation (1), with a thermal diffusivity β equal to

$$\beta = \kappa/c \qquad \Longleftrightarrow \qquad \kappa = c\beta. \tag{8}$$

The obtained relation is valid if we neglect the temperature dependence of the coefficients κ and c. This is permissible if the temperature variations are small (compared to its absolute value) or the dependence of the coefficients on temperature is weak (as will be implemented on the molecular dynamics model under consideration). Thus, after determining the thermal diffusivity β from Eq. (6) according to the simulation results, the thermal conductivity coefficient is determined by Eq. (8). Specific expressions for the heat capacity c will be given in the next section.

2 Computer modeling

Consider the material under study by a set of particles interacting through a pair potential $\Pi(r)$. The equations of motion of particles have the form

$$m\ddot{\mathbf{r}}_k = \sum_{n=1}^{N} \frac{f(|\mathbf{r}_k - \mathbf{r}_n|)}{|\mathbf{r}_k - \mathbf{r}_n|} (\mathbf{r}_k - \mathbf{r}_n) - \lambda (\dot{r}_k - \dot{r}_n), \tag{9}$$

where $\mathbf{r}_k$ is the radius vector of the k-th particle, m is the particle mass, N is the total number of particles in the system, and $f(r) = -\Pi'(r)$ is the force of interaction between two particles. We introduce the following notation: a is the equilibrium distance between two particles, $D = |\Pi(a)|$ is the binding energy, $C = \Pi''(a) \equiv -f'(a)$ is the stiffness of the interatomic bond in the equilibrium position, $v_d = \sqrt{2D/m}$ is the dissociation velocity (minimum speed required to exit the potential field), $\tau_0 = 2\pi\sqrt{m/C}$ is the period of oscillation of mass m under the action of a linear force with stiffness C. Additional information on the modeling method used can be found in [33, 34]. Also λ is a coefficient depending on temperature. In the simplest case, $\lambda = \zeta(T - T_0)$, where ζ is a constant characterizing the heating intensity of the system; T and T_0 are the actual and required temperatures at a given point in space. It is possible to use other methods of specifying the coefficient k, for example, as in the Noze-Hoover's thermostat [35]. When the system is brought to the desired thermal state, the term proportional to λ is removed and the process of natural temperature equalization begins, which is used to determine the thermal conductivity of the sample.

Consider the classic Lennard-Jones potential:

$$\Pi_{LJ}(r) = D\left[\left(\frac{a}{r}\right)^{12} - 2\left(\frac{a}{r}\right)^{6}\right], \tag{10}$$

$$f_{LJ}(r) = -\Pi'_{LJ}(r) = \frac{12D}{a}\left[\left(\frac{a}{r}\right)^{13} - \left(\frac{a}{r}\right)^{7}\right], \tag{11}$$

where D and a are the energy and length of the bond. For the Lennard-Jones potential, the stiffness C and the binding energy D satisfy the relation $C = 72D/a^2$; force (11) reaches its minimum value when $r = b = \sqrt[6]{13/7}$, where b is the distance corresponding to the strength of the interatomic bond. For simulations the modified Lennard-Jones potential is used:

$$f(r) = \begin{bmatrix} f_{LJ}(r), & 0 < r \leq b, \\ k(r)f_{LJ}(r), & b < r \leq a_{\text{cut}}; \end{bmatrix} \tag{12}$$

where b is the distance corresponding to the Lennard-Jones interatomic bond strength, a_{cut} is the cutoff radius (for $r > a_{\text{cut}}$ the interaction force vanishes). The coefficient $k(r)$ is the modifying function:

$$k(r) = \left[1 - \left(\frac{r^2 - b^2}{a_{\text{cut}}^2 - b^2}\right)^2\right]^2. \tag{13}$$

The cutoff radius is given by the relation $a_{\text{cut}} = 1.4a$, in this case only the nearest neighbors in the close-packed lattice will interact with each other. Note the thermal conductivity in the Lennard-Jones model material is considered here, not the behavior of a particular real material, and for these purposes the proposed simplified potentials are sufficient. However, these results can be further transferred to more complex potentials, which more accurately describe the actual materials. Moreover, as it will be shown below, the empirical relations obtained on the model material describes well the processes in such real materials as isotopically enriched diamond.

3 Computer experiments

A crystal lattice with a uniform distribution of defects is considered. The role of defects is played by vacancies or the inclusion of atoms of greater mass (see Fig. 1). The density of defects will be denoted by the parameter p, which determines the ratio of the number of defects to the number of nodes in the lattice. Periodic boundary conditions are imposed on all sample boundaries. A rectangular sample of a material with an initial temperature distribution in the form (2) is considered, where the x axis is directed along one of the edges of the parallelepiped, L is the sample length along this axis, and the sample sizes in orthogonal directions are equal to $L/4$. The particles are located at the nodes of a close-packed lattice, triangular in two-dimensional and face-centered cubic (FCC) in the three-dimensional case.
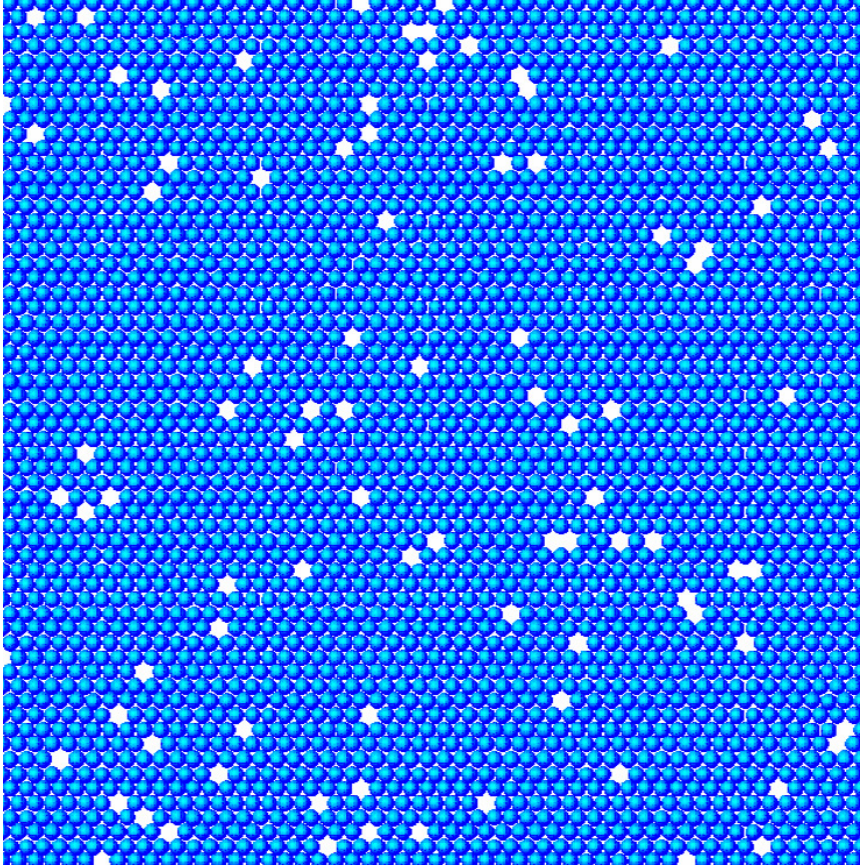
Fig. 1 *An element of a 2D single crystal with a specified distribution of defects. Two-dimensional crystal is presented for clarity, three-dimensional models are also used for the computations.*

The kinetic temperature is

$$\frac{d}{2}\,k_B T = E_K, \qquad E_K = \left\langle \frac{mv^2}{2} \right\rangle, \tag{14}$$

where d is the dimension of the space (2 or 3), k_B is the Boltzmann constant, E_K is the average kinetic energy of a particle, $\langle ... \rangle$ is the averaging over a certain set of particles (in this paper, we use the averaging over a layer of particles perpendicular to the x axis). The average temperature of the system is assumed to be $T_1 = 3.2 \cdot 10^{-5} T_d$, where $T_d = v_d^2/2$, $v_d = \sqrt{2D/m}$ is the dissociation velocity, m is the mass of a particle. The amplitude of temperature deviations is taken equal to $T_2 = (2/3)T_1$. The heat capacity of the considered computer material is

$$U = \frac{E_K + E_\Pi}{V_0} \approx \frac{2E_K}{V_0} \qquad \Longrightarrow \qquad c = \frac{U}{T} = \frac{d\,k_B}{2V_0}, \tag{15}$$

where V_0 is the volume of the unit cell of the crystal lattice; E_Π is the potential energy of a particle; U is the specific thermal energy per unit volume of material. Here, the approximate equality of the kinetic and potential energies is used (fair, according to the virial theorem, for sufficiently low temperatures at which the nonlinear interatomic interaction can be neglected). Variations in the heat capacity due to quantum effects are not taken into account in this model. The unit cell volume for close-packed lattices is determined by

$$V_0 = \frac{\sqrt{5-d}}{2}\,a^d, \tag{16}$$

where d is the dimension of the space (2 or 3 in our case), a is the lattice spacing. Using Eqs. (8), (15) and (16), we obtain the following relation between thermal conductivity κ and thermal diffusivity β:

$$\kappa = \frac{d\,k_B}{\sqrt{5-d}\,\,a^d}\,\beta. \tag{17}$$

At the initial time, the particles are located near the sites of the crystal lattice, while they are given random deviations from the equilibrium position. The initial velocities of the particles are chosen randomly so that their dispersion corresponds to the initial value of the kinetic temperature. Random initial displacements are chosen from the condition of equality of potential and kinetic energies of thermal motion. When assigning random variables, a uniform statistical distribution is chosen, however, the Maxwell distribution for velocities and coordinates is established rather quickly (within tens of τ_0).

3.1 Lattice with vacancies

Based on the computation results, graphs of the dependence of the thermal diffusivity coefficient β on the density of defects in the material for the two-dimensional and three-dimensional cases were constructed — see Figs. 2–3. It is seen that the coefficient of thermal diffusivity strongly depends on the number of defects and
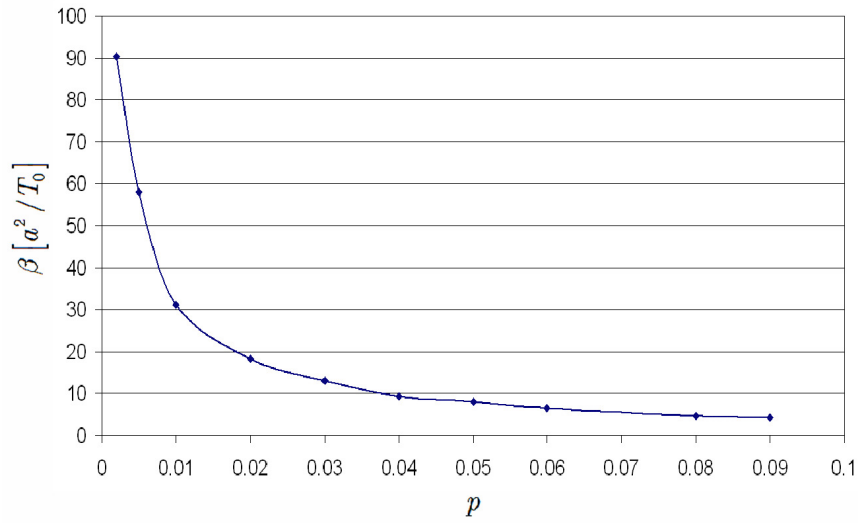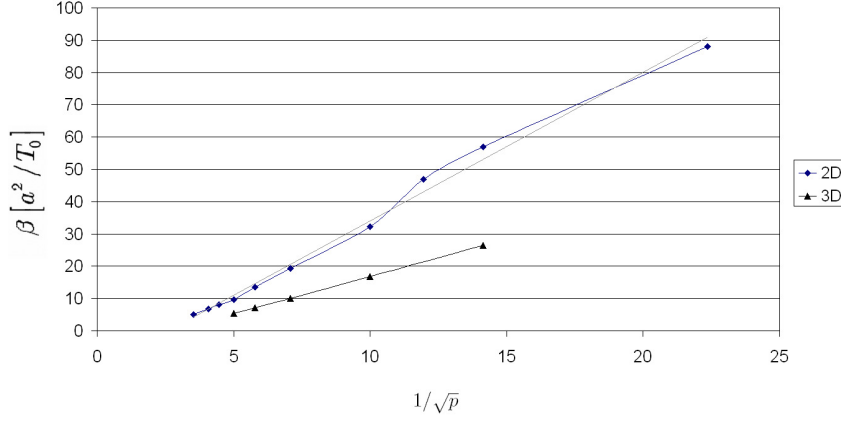
Fig. 2 *The dependence of the thermal diffusivity β on the defect density p for a two-dimensional crystal, obtained from the simulation results.*
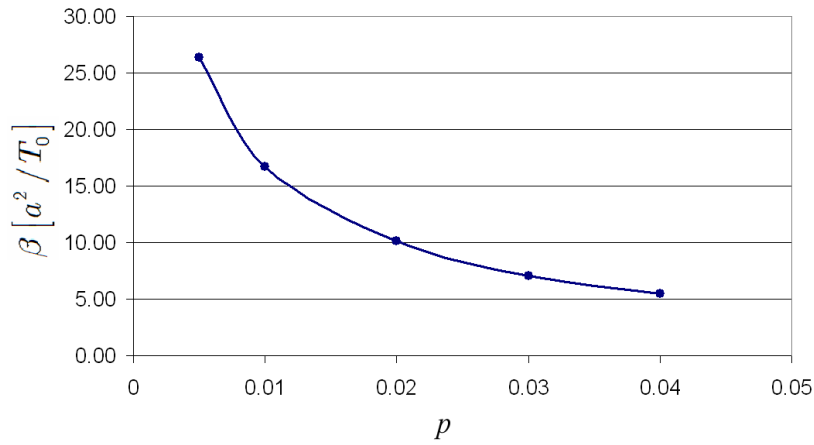
Fig. 3 *The dependence of the thermal diffusivity β on the defect density p for a three-dimensional crystal, obtained from the simulation results.*

this dependence is quite definite. Numerical analysis has shown that the dependence with a high degree of accuracy is inversely proportional to the root of the porosity.

Figure 4 shows graphs of the dependence of the thermal diffusivity on $1/\sqrt{p}$. It is noteworthy that the resulting dependencies are linear to within small de-

Fig. 4 *The change in the thermal diffusivity β depending on the value of $1/\sqrt{p}$, where p is the density of the lattice defects.*

viations, probably caused by a lack of statistical data. For the two-dimensional case, these deviations are so small that the depicted trend line is visually indistinguishable from the dependency graph itself. Based on these results, the following approximation of the $\beta(p)$ dependence can be obtained:

$$\beta = A \left(\frac{1}{\sqrt{p}} - \frac{1}{\sqrt{p_0}} \right),$$ (18)

where A is the dimensional coefficient, p_0 is the critical value of the density of defects, at which the thermal conductivity vanishes. The values of these two parameters obtained from the computer simulations for two-dimensional and three-dimensional crystals are given in Table. 1.

Parameter	2D	3D
$A \left[a^2/\tau_0 \right]$	4.67	2.29
p_0	0.131	0.144

**Table 1** *The values of the coefficients A and p_0 for the dependence (18).*

3.2 Lattice with atoms of different mass

We consider the inclusions of particles whose mass is two times greater than masses of the other particles of the system. The technique of molecular dynamics simulation is similar to the previous case; a three-dimensional crystal with a FCC lattice is investigated. The simulation results are marked with rhombic markers in Fig. 5. All possible concentrations — from zero to 100% are considered. The solid line represents the approximate dependence in the form

$$\beta = A \frac{1}{\sqrt{p}} + B \frac{1}{\sqrt{1-p}} + C,$$ (19)

with selected least squares coefficients A, B, C. In contrast to the previous case, when vacancies appeared as defects, the resulting dependence is non-monotonic and has a minimum. From the graph it is seen that with a small number of inclusions (both small and large masses), an increase in their concentration leads to a sharp decrease in thermal conductivity (as in the case of vacancies). However, with an approximate equality of the number of light and heavy particles, the minimum value of thermal conductivity is reached. The chosen approximation (19) describes the dependence under consideration up to the accuracy of the simulation data and can be interpreted as a generalization of the dependence (18).
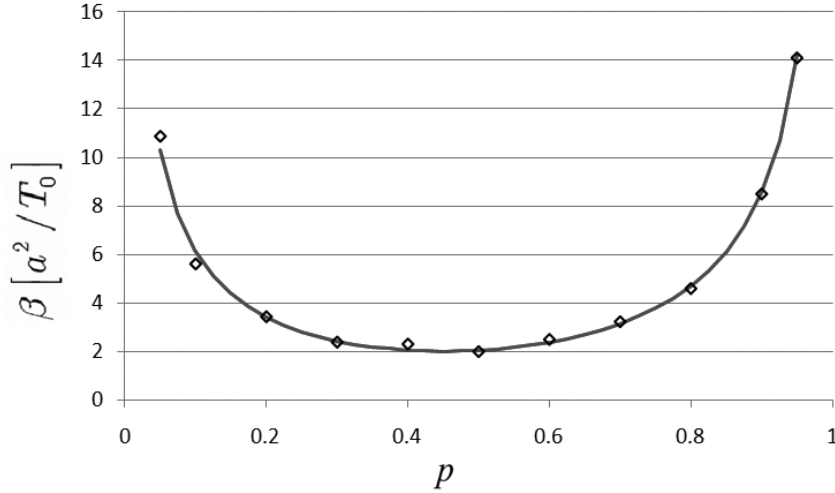

Fig. 5 *The change in the thermal diffusivity β depending on the value of p, which is the ratio of the number of particles with double mass to the total number of particles.*

3.3 Comparison with experimental data

The thermal conductivity of a diamond single crystal with defects in the form of carbon isotope inclusions^{13}C was studied experimentally in Refs. [28–31]. In view of the high purity of diamond crystals, experimental data are well suited for comparison with our numerical results. One can see the change in the thermal conductivity coefficient K depending on the density of defects in the crystal lattice p in Fig. 6. The solid line shows the empirical dependence for the coefficient of thermal conductivity, similar to Eq. (19), with the coefficients obtained using the least squares method:

$$\kappa = \kappa_0 \left(\frac{1}{\sqrt{p}} + \frac{1}{\sqrt{1-p}} \right), \tag{20}$$

where κ is the thermal conductivity coefficient, p is the ratio of the number of isotopes ^{13}C to the total number of atoms, $\kappa_0 = 2.45$ W/(cm · K) is a dimensional parameter. The dependency (20) is a particular form of the expression (19)
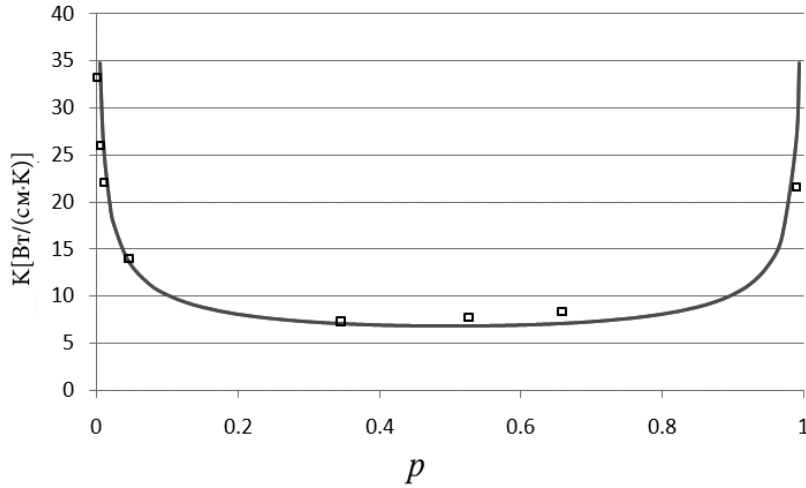
Fig. 6 *The change in the thermal conductivity coefficient κ depending on the density of defects in the crystal lattice p. Rectangular markers correspond to the experimental data, solid line is the empirical dependence.*

rewritten for the thermal conductivity coefficient at $A = B$, $C = 0$. The use of expression (19) for the heat conductivity is possible since coefficients β and κ are proportional according to relation (17).

Thus, the empirical dependence obtained for the Lennard-Jones model material in the form (19) can be generalized to the case of real material. In addition, the expression (20) gives a good approximation to the experimental data for a diamond single crystal with the inclusion of the ^{13}C isotopes presented in Refs. [28–31].

4 Conclusions

According to the results of the computer experiments, the thermal diffusivity coefficient was measured at various density of defects of different nature (vacancies, mass inclusions). Based on these data, a general empirical dependence of the coefficient of thermal diffusivity on the density of defects was obtained in the form (19). For the particular case of vacancies the dependence takes the form (18). Comparison with the results of the nature experiments for diamond single crystal with ^{13}C isotope inclusions demonstrates excellent fitting of the obtained empirical dependence (19) the experimental data. These results may be useful in relation to the nanotechnology involving heat transfer processes in high purity nanostructures [36–39].

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