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COMPUTER EXPERIMENTS ON PROPAGATION AND ELASTIC SCATTERING OF BEAMS OF DOWN-CONVERTING PHONONS

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Abstract. We present the program *MCAnScat* which simulates propagation of beams of down-converting phonons in anisotropic cubic and isotropic media containing point mass defects. It is assumed that the excitation the phonon subsystem is low-level. The program produces time-of-flight spectrograms and phonon energy and quasi-momentum focusing patterns for samples having the form of a rectangular parallelepiped, as well as for cylindric and spherical specimens. Wave vectors of beam phonons belong to body angles ranging from 4π to zero. The axes of corresponding cones are arbitrarily oriented. When down-conversion processes are excluded the outcomes of experiments on initial spatially homogeneous states and on diffusive propagation of phonons are compared with exact results obtained for isotropic and cubic media. As an example of application of *MCAnScat* we study ballistic and diffusive propagation of beams of phonons in GaAs. The obtained results are in excellent agreement with theoretical and experimental findings.

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I. INTRODUCTION

During the last three decades the spectroscopy of time-of-flight and of phonon images has been developed. For their purposes beams of phonons at low temperatures are used. These beams propagate in generally anisotropic media and are scattered by defects and other quasi-particles. For the study of the problem of such complexity the traditional approach, involving explicit solution of the Boltzmann equation, represents a formidable problem, and we have chosen, instead, to use the Monte Carlo method.

Generally, propagating phonons are scattered by defects and undergo the splitting and coalescence anharmonic processes (cf. [1-7]). However, for the ambient temperature T much lower than the Debye temperature θ_D (i.e. for very small densities of the gas of thermal phonons [7] coalescence processes can be neglected in comparison with the spontaneous splitting processes. *Here we consider only the scattering and down-conversion (spontaneous splitting)*

processes of phonons of the beam. As a result of these processes the number of phonons in a given state diminishes, and hence they provide the mechanism of decay of phonons.

In our previous paper we considered the program *MCFoc* for computer experiments with beams of phonons which propagate ballistically (i.e. without collisions and splitting events) in anisotropic crystalline media [8],

Our present program *MCAnScat (Mo*nte Carlo simulation of *AN*isotropic *SCATtering)* allows for performing computer experiments on beams of down-converting, long wavelength acoustic phonons (LAPs for short) propagating in anisotropic crystalline media containing point mass defects (PDMs).

Furthermore, we previously obtained a number of exact results for the problem of scattering of long wavelength phonons by point mass defects [9-13], Therefore, unlike Lax et al [1] we do not use concepts that arose from other models of kinetics (e.g. the *Milne isotropic* problem in astrophysics) and put the study of the influence of elastic anisotropy on propagation and scattering of phonons by PMDs (cf. [14]) on the firm ground. We consider here the situation when the down-conversion processes are much less frequent than the processes of elastic scattering. Recent experiments on diffusive propagation of phonon beams in yttrium aluminum garnets containing rare earth substitutional atoms [15] performed at helium temperatures made it evident that physical conditions which correspond to such restricted computer experiments can be achieved.

Since in our previous paper [8] we presented a rather detailed description of the problems of generation and detection of phonon pulses as well as the properties of LAPs, in the first part of the present paper we confine ourselves mainly to the short description of scattering of phonons by point mass defects. We also describe spontaneous splitting processes of phonons.

The problem of anisotropic propagation and elastic scattering of down-converting phonons shares the general features of beams of elementary particles. Therefore, we expect that our particular problem is of interest to quite a wide audience.

II. OBJECT ORIENTED PROGRAMMING

Experience tells us that at the beginning of a project of a software development the programmer does not really understand the full implications and the scope of the project. As a rule, up to 40% of maintenance costs (including changes in the product following initial release) result from unforeseen changes in user requirements.

We frequently experienced such changes working with program of Monte Carlo simulation of propagation and scattering of beams of particles and quasi-particles [8, 16]. The demands of the experimenters grow as a result of improvements in the equipment and, as new scientific problems arise, theoreticians have to check new ideas and new situations. The goal of our software should not only be correctness, the ability to match the requirements and specifications, but also flexibility and expendability, along with the ability to adapt to changes in the specifications. Another goal is to develop a software which is reusable because it is not tightly

coupled to a particular project. Reusability can lead to significant improvements in overall productivity, not necessarily for a single project, but by applying the same software to multiple projects.

All the above demands meet the requirements of object-oriented programming (OOP) and C++ programing language as the most familiar implementation of OOP (cf. Sect. VI).

HI. REAL-LIFE VERSUS COMPUTER EXPERIMENTS ON BEAMS OF PHONONS

A complete description of experiments with beams of phonons can be found in the book by Wolfe [17]. Generally one can distinguish two kinds of experiments with the use of phonon beams - namely transmission and reflection experiments. In the transmission experiments one studies crystalline anisotropy and interaction of injected phonons with defects of ideal crystalline structure and with thermal quasi-particles present in the medium as well as the internal dynamics of phonons (e.g. the phonon down-conversion processes). The phonon reflection experiments allow one to study interaction of phonons with boundaries and interfaces (cf. [18]).

In our paper we confine ourselves to the low-temperature transmission experiments performed on good quality massive specimens which may contain a small amount of isotope or substitutional atoms. In such conditions one can neglect the boundary scattering. Non-equilibrium phonons are elastically scattered and undergo anharmonic down-conversion processes - mostly splitting of phonons into pairs of daughter phonons. In the case of long wavelength acoustic phonons, considered here, the dynamics of injected phonons depends on the mass density, linear and nonlinear elastic properties of the crystalline media and characteristics of scattering centers. The set of these characteristics is attributed to the medium.

As a rule specimens used in real-life experiments have the form of rectangular parallelepiped [17] or discs [19]. In early experiments Hensel and Dynes [20] used the sample in the shape of a hemi-cylinder. The typical characteristic length of samples (e.g. the thickness of a disc) ranges from 0.1 to 1 cm. The experimenter should select the kind of specimen and properly cut it, i.e. choose the orientation of boundaries and axes with respect to crystalline axes.

The mentioned properties characterize specimens. In our program to the specimen made of the chosen medium there corresponds an **object** specimen. This object animates phonons — it moves and scatters them and governs the down-conversion processes which they undergo.

Phonons are injected into the specimen by a source which, as a rule, is placed on one of specimen boundaries. In experiments with beams of elementary particles phonons are generated also inside specimens. Phonons can be radiated by current-driven metallic films, by photo-excited regions of boundaries, by tunnel junctions and by excited $2D$ gases of carriers. The two former types of sources are very efficient and have a broad distribution of energies. The latter type of generators give quasi-monochromatic beams characterized by the linear frequency ν.

Electrons of electrically-driven metallic films relax *via* fast processes of phonon radiation. Since the process of transmission of these phonons from metal to crystalline specimen is rather

slow, the combined system of electrons and phonons reaches "local" equilibrium state with temperature T_H different from the ambient temperature T. The frequency distribution function $F(\nu, T_H)$ of these phonons depends on phase ($cj^{(h)}$) and the Debye ($c_D^{(h)}$) velocities of the heater material, namely

$$F(\nu, T_H) = \left(\frac{c_D^{(h)}}{c_j^{(h)}} \right)^3 \nu^2 f_0 \left(\frac{h\nu}{k_B T_H} \right),$$

where f_0 is the Planck function. The non-equilibrium phonons are transmitted to the specimen.

Generation of phonons by photo-excitation is also a complicated multi-step physical process and the spectral composition of non-equilibrium phonons is, as yet, poorly understood.

Sources can be fixed (e.g. a Joule-heated metallic films or Josephson junctions deposited onto one side of the specimen) or movable (e.g. excited regions of specimen surface or a metallic film).

We see that sources are characterized by their linear dimensions and the spectral composition of radiated phonons. If the source is placed on boundaries, it is additionally designated by the vector $\hat{\mathbf{n}}$ normal to the surface. Sources placed on boundaries radiate phonons into the body angle $d\Omega_s = 2\pi$. In real experiments, in some restricted way, the angle $d\Omega_s$ can be controlled by "slots" in the ciystal [21], which physically block a selected part of the phonon flux. In our computer experiments $0 < d\Omega_s \leq 2\pi$. In *MCAnScat* program the source of phonons is represented by the **object** source. It creates phonons in a probabilistic way attributing them the suitable characteristics (frequencies, polarization, wave vectors and coordinates).

Phonons generated by the source move in the medium towards a detector. It may be a fast bolometer, such as a super-conducting thin film at its transition temperature or a Josephson junction. Low-dimensional gases of charge carriers are sensitive to the quasi-momenta of phonons (cf. [22]). We shall call them phonon anemometers. With a few exceptions (CdS detectors and clouds of excitons) detectors are immovable. Therefore, in our computer experiments detectors are fixed and characterized by a set of quantities analogous to those describing sources.

Since the detector position is fixed, the direction of propagation of phonons changes when source moves across the surface. Due to the anisotropy of the medium, currents of energy and quasi-momentum which fall onto the detector depend on direction of propagation and in our experiments they are recorded as functions of source coordinates. In this way one obtains phonon images of cubic crystals (patterns of density of energy and of a selected component η of quasi-momentum density). In computer experiments the detector is represented by a rectangular matrix consisting of $n \times m$ cells - elementaiy detectors (each of them corresponds to a detector used in real-life experiments). Each elementary detector integrates the incoming fluxes over the detector surface area and eventually over time.

Additionally, for a selected position of both the source and the detector one can study the time dependence of the detector signal (time-of-flight spectrograms). In computer experiments the device "detector" is represented by the **object** detector.

The **object** phonon represents a "quasi-particle phonon" with the characteristics of a phonon provided by the source. The source establishes the remaining phonon characteristics (e.g. the phase and group velocities and polarization vectors). Phonon does not allow propagation outside the specimen.

The role of a laboratory assistant is taken by the **object** parser, which is responsible for accepting data introduced by the user and for transforming them into the list of jobs. The parser in our program is declared as an automatic object which supplies lists of data used for creation the **object** experiment in the loop until the list of jobs is exhausted. Additionally, the experiment contains the counter of phonons.

III.1. Relaxation of weakly and strongly excited phonon systems

Sources of phonons excite the phonon subsystem of the specimen, which initially is in the equilibrium state characterized by the temperature T and by the Planck distribution function $f_0(h\nu/k_BT)$. Consider non-equilibrium phonons characterized by the frequency ν^* containing energy, the density of which is E^* [6], The phonon subsystem is weakly excited when $h\nu^* \lesssim k_BT$ and E^* is small compared to the energy density of thermal phonons $E(T)$. If $h\nu^* \gg k_BT$ and (or) $E^* \gg E(T)$ phonons are strongly excited and, in contrast to weakly excited ones, their distribution function f is far from Planckian. In this paper we consider only strongly excited phonon gases and assume that the ambient temperature is low (i.e. $T \ll h\nu^*/k_B \ll \theta_D$).

The probability density of various phonon processes depend on their frequency v* and ambient temperature T, and is characterized by the inverse relaxation times $\tau^{-1}(\nu^*)$. We shall consider here decay and background scattering processes involving three phonons and elastic scattering processes by point mass defects. The related relaxation rates were collected by Levinson in the form of a table [6], which we reproduce here (Table I).

Table I. Relaxation rates for various phonon processes

Process		τ^{-1}	Frequencies of contributing phonons
Decay			
spontaneous background	a) $h\nu^* \gg k_BT$	$(\nu^*)^5$ $T^3(\nu^*)^2$	$\nu^* \simeq \nu' \simeq \nu''$ $h\nu' \simeq k_BT$, $\nu'' \simeq \nu^*$ or $\nu' \simeq \nu^*$, $h\nu'' \simeq k_BT$
induced	b) $h\nu^* \ll k_BT$	$T(\nu^*)^4$	$h\nu' \simeq h\nu'' \simeq k_BT$
Background scattering			
	a) $h\nu^* \gg k_BT$	$T^3(\nu^*)^2$	$\nu' \simeq \nu^*$, $h\nu'' \simeq k_BT$
	b) $h\nu^* \ll k_BT$	$T^4\nu^*$	$h\nu' \simeq h\nu'' \simeq k_BT$
elastic scattering		$(\nu^*)^4$	

IV. PROPERTIES OF ISOTROPIC AND CUBIC MEDIA

For long wavelength phonons a crystalline medium can be treated as an anisotropic, generally nonlinear, elastic medium in which point mass defects are embedded. These media are characterized by the mass density ρ and a suitable set of elastic constants (EC); namely by the second-order (linear EC) - $C_{\alpha\mu,\ \beta\nu}$ and the third-order (the first of the set of nonlinear EC) – $C_{\alpha 1\mu 1,\,\alpha 2\mu 2,\,\alpha 3\mu 3}$ where $\alpha_1, \ldots, \mu_3 = 1, 2, 3$. The EC are components of tensors of elastic constants $\mathcal{C}_2$ and $\mathcal{C}_3$. When permutations of the tensor indices are taken into account the representation to which $\mathcal{C}_2$ belongs is $[[V^2]^2]$, and $\mathcal{C}_3$ belongs to $[[V^2]^3]$ (cf. [23]).

Consider a deformed medium characterized by the nonlinear symmetric deformation tensor η with components

$$\eta_{\alpha\mu}(\mathbf{r}) = \frac{1}{2}\left[u_{\alpha\mu}(\mathbf{r}) + u_{\mu\alpha}(\mathbf{r}) + \sum_{\gamma=1}^{3} u_{\gamma\alpha}(\mathbf{r})\, u_{\gamma\mu}(\mathbf{r})\right],$$

where $\mathbf{r}$ is the radius vector of a small volume element of the medium. The elements $u_{\alpha\mu}(\mathbf{r})$ are the strain fields $u_{\alpha\mu}(\mathbf{r}) = \partial u_\alpha(\mathbf{r})/\partial r_\mu$.

The deformation energy $H_d^{(V)}$ of a medium filling the volume V is

$$H_{def}^{(V)} = \int_V d^3\mathbf{r}\left[\frac{1}{2!}\sum_{\{\alpha,\,\mu\}} C_{\alpha_1\mu_1,\,\alpha_2\mu_2}\,\eta_{\alpha_1\mu_1}(\mathbf{r})\,\eta_{\alpha_2\mu_2}(\mathbf{r}) + \right.$$
$$\left. + \frac{1}{3!}\sum_{\{\alpha,\,\mu\}} C_{\alpha_1\mu_1,\,\alpha_2\mu_2,\,\alpha_3\mu_3}\eta_{\alpha_1\mu_1}(\mathbf{r})\,\eta_{\alpha_2\mu_2}(\mathbf{r})\,\eta_{\alpha_3\mu_3}(\mathbf{r}) + \ldots\right]. \tag{1}$$

The dominating, second-order ECs define the frequencies of long wavelength acoustic phonons. The third-order ECs give the main contribution to the probability densities of various three-phonon anharmonic (down-conversion and coalescence) processes of LAPs. We shall include here only the spontaneous down-conversion processes.

IV. 1. Second-order elastic constants for cubic and isotropic media

IV. 1.1. Cubic media

In place of pairs of Greek, indices we shall use Latin indices $i,j,\ldots = 1,\ldots 6$ (cf. [24]). For isotropic media the set of linear elastic constants contains two elastic constants C_{11} and C_{12}. Cubic media are additionally characterized by C_{44}. For cubic media the tensor C_2 contains three terms

$$\mathcal{C} = C_J\mathcal{J} + C_L\mathcal{K} + K\mathcal{M} \tag{2}$$

where $C_J = (C_{11} + 2C_{12})$, $C_L = 2C_{44}$, $K = (C_{11} - C_{12} - 2C_{44})$ is the elastic anisotropy parameter ($K = 0$ for isotropic media) and

$$\mathcal{M} = (\mathcal{S} - \mathcal{J}), \quad \mathcal{K} = (\mathcal{I} - \mathcal{J}),$$

$$J^{\alpha\mu,\beta\nu} = \frac{1}{3}\delta_{\alpha,\mu}\,\delta_{\beta,\nu}, \qquad I^{\alpha\mu,\beta\nu} = \frac{1}{2}\left(\delta_{\alpha,\beta}\delta_{\mu,\nu} + \delta_{\alpha,\nu}\delta_{\beta,\mu}\right). \tag{3}$$

The tensor $\boldsymbol{S}$ consists of products of components of three unit vectors $\hat{\mathbf{a}}, \hat{\mathbf{b}}, \hat{\mathbf{c}}$ directed along three fourfold axes of symmetry

$$\boldsymbol{S} = \left(\hat{\mathbf{a}}\otimes\hat{\mathbf{a}}\otimes\hat{\mathbf{a}}\otimes\hat{\mathbf{a}} + \hat{\mathbf{b}}\otimes\hat{\mathbf{b}}\otimes\hat{\mathbf{b}}\otimes\hat{\mathbf{b}} + \hat{\mathbf{c}}\otimes\hat{\mathbf{c}}\otimes\hat{\mathbf{c}}\otimes\hat{\mathbf{c}}\right). \tag{4}$$

The tensor $(\hat{\mathbf{a}}\otimes\hat{\mathbf{a}}\otimes\hat{\mathbf{a}}\otimes\hat{\mathbf{a}})$ has components $(\hat{\mathbf{a}}\otimes\hat{\mathbf{a}}\otimes\hat{\mathbf{a}}\otimes\hat{\mathbf{a}})_{\alpha\mu\beta\nu} = \hat{a}_\alpha\,\hat{a}_\mu\,\hat{a}_\beta\,\hat{a}_\nu$. The mechanical stability conditions impose some restrictions on parameters C_{11}, C_{12}, C_{44}, they obey three inequalities [24],

We are able to study processes in which phonons down convert to pairs of daughter phonons only in effective isotropic media corresponding to cubic ones. Therefore we shall find elasticity parameters for such effective isotropic media. Averaging components of the tensor S over all directions of vectors $\hat{\mathbf{a}}, \hat{\mathbf{b}}$ and $\hat{\mathbf{c}}$ and using the identity valid for each of three elements of $\boldsymbol{S}$ [24], e.g.

$$\langle a_\alpha a_\mu a_\beta a_\nu\rangle = \frac{1}{15}\left(\delta_{\alpha,\mu}\delta_{\beta,\nu} + \delta_{\alpha,\beta}\delta_{\mu,\nu} + \delta_{\alpha,\nu}\delta_{\beta,\mu}\right).$$

we obtain

$$\mathcal{C}_{ef}^{(is)} = C_J^{(ef)}\mathcal{J} + C_K^{(ef)}K, \tag{5}$$

where

$$C_J^{(ef)} = C_J, \qquad C_K^{(ef)} = C_L + \frac{2}{5}K. \tag{6}$$

From mentioned inequalities it follows that the tensor $\mathcal{C}_{ef}^{(is)}$ is positive, i.e. effective media are mechanically stable (cf. also [25]), i.e. $C_J > 0$ and $C_K^{(ef)} > 0$.

In our previous paper [25,26] we applied this method of derivation of the second and third order elastic constants for effective isotropic media corresponding to all crystal classes and listed them. A different method of obtaining effective elastic constants was proposed by Fedorov [24] (cf. also [27]).

IV.1.2. Isotropic media

For an isotropic elastic medium the tensor of second order elastic constants has the same structure as $\mathcal{C}_{ef}^{(is)}$ (5) [28]

$$C = C_J\mathcal{J} + C_K\mathcal{K}, \tag{7}$$

where the coefficients C_J, C_K can be expressed by C_{11} and C_{12}

$$C_J = (C_{11} + 2C_{12}), \qquad C_K = (C_{11} - C_{12}). \tag{8}$$

An elastic medium is mechanically stable when $C_J > 0$, $C_K > 0$.

IV.2. Propagation of acoustic waves in cubic and isotropic media

IV.2.1. Isotropic and effective isotropic media

Consider an acoustic wave with the propagation vector $\mathbf{k} = \hat{\mathbf{k}}k$, where $k = |\mathbf{k}|$ and $\hat{\mathbf{k}} = \mathbf{k}/k$. For isotropic media (including the effective ones) the propagation matrix $\Lambda_{is}(\hat{\mathbf{k}})$ with elements $\rho^{-1}\Sigma_{\mu,\nu}C_{\alpha\mu\beta\nu}\hat{k}_\mu\hat{k}_\nu$ has a very simple form (cf. [24])

$$\Lambda_{is}(\hat{\mathbf{k}}) = \frac{1}{3\rho}\left(C_J + \frac{1}{2}C_K^{(\sigma)}\right)\hat{\mathbf{k}}\otimes\hat{\mathbf{k}} + \frac{1}{2\rho}C_K^{(\sigma)}\mathbf{I}_2, \tag{9}$$

where $\mathbf{I}_2$ has the elements $\delta_{\alpha,\beta}$ and σ= isotr, eff isotr. Therefore, it is obvious that $\mathbf{e}_0 = \hat{\mathbf{k}}$ is the eigenvector of $\Lambda_{is}(\hat{\mathbf{k}})$ corresponding to the eigenvalue c_0 equal

$$c_0 = c_l \equiv \sqrt{\frac{C_J + 2C_K}{3\rho}} = \sqrt{\frac{C_{11}}{\rho}} = \sqrt{\frac{\lambda + 2\mu}{\rho}}. \tag{10}$$

Any pair of mutually perpendicular eigenvectors $\mathbf{e}_1$, $\mathbf{e}_2$, which are also perpendicular to $\hat{\mathbf{k}}$, represents the remaining two eigenvectors. They correspond to the two degenerate eigenvalues

$$c_1 = c_2 = c_t \equiv \sqrt{\frac{C_K}{2\rho}} = \sqrt{\frac{C_{11} - C_{12}}{2\rho}} = \sqrt{\frac{\mu}{\rho}}, \tag{11}$$

where λ and μ are the Lamé coefficients

$$\lambda = C_{12}, \qquad \mu = \frac{1}{2}(C_{11} - C_{12}).$$

For effective isotropic elastic media one gets (cf. Tamura [37])

$$\lambda^{(ef)} = \frac{1}{5}(C_{11} + 4C_{12} - 2C_{44}), \qquad \mu^{(ef)} = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}). \tag{12}$$

As a result of the positivity of $\Lambda(\hat{\mathbf{k}})$ the eigenvalues c_l and c_t (called the phase velocities) are real. For effective elastic medium we obtain

$$c_l^{(ef)} = \sqrt{\frac{1}{5\rho}(3C_{11} + 2C_{12} + 4C_{44})}, \qquad c_t^{(ef)} = \sqrt{\frac{1}{5\rho}(C_{11} - C_{12} + 3C_{44})}. \tag{13}$$

Since elastic constants obey stability conditions these quantities are also real for all cubic media.

IV.2.2. Cubic media

Apart of a scaling factor $C_1 = (C_{11} + 2C_{44})$, phase velocities and polarization vectors depend only on dimensionless parameters $s_2 = C_2/C_1$ and $s_3 = K/C_1$ where $C_2 = (C_{11} - C_{44})$ (cf. [12,19]).

Introduce the velocity $c = \sqrt{C_1/3\rho}$. The phase and components of the group velocities also can be expressed in terms of c and functions of $\hat{K}$, viz.

$$c(\hat{K}) = c\tilde{c}(\hat{K}), \qquad v_\alpha(\hat{K}) = c\,\tilde{v}_\alpha(\hat{K}), \qquad (\alpha = 1,2,3). \tag{14}$$

The dimensionless quantities $\tilde{c}(\hat{K})$, $\tilde{v}_\alpha(\hat{K})$ $(\alpha = 1, 2, 3)$ depend on the components of $\hat{k}$ and s_2, s_3 *via* several functions introduced by Every [29]

$$G(\hat{\mathbf{k}}) = s_1^2[s_2^2 - 3s_3[2s_2 - s_3)]\mathcal{P}(\hat{\mathbf{k}}) \equiv s_1^2 G_0(\hat{\mathbf{k}}), \tag{15}$$

$$\begin{aligned} H(\hat{\mathbf{k}}) &= s_1^3\left[s_2^3 - \frac{9}{2}s_2 s_3(2s_2 - s_3)\right]\mathcal{P}(\hat{\mathbf{k}}) + \\ &+ \frac{27}{2}s_3^2(3s_2 - 2s_3)\mathcal{Q}(\hat{\mathbf{k}}) \equiv s_1^3 H_0(\hat{\mathbf{k}}), \end{aligned} \tag{16}$$

and

$$\psi(\hat{\mathbf{k}}) = \frac{1}{3}\arccos\left[H(\hat{\mathbf{k}})/G^{3/2}(\hat{\mathbf{k}})\right] = \frac{1}{3}\arccos\left[H_0(\hat{\mathbf{k}})/G_0^{3/2}(\hat{\mathbf{k}})\right], \tag{17}$$

where

$$\mathcal{P}(\hat{\mathbf{k}}) = \hat{k}_1^2\hat{k}_2^2 + \hat{k}_2^2\hat{k}_3^2 + \hat{k}_3^2\hat{k}_1^2, \qquad \text{and} \qquad \mathcal{Q}(\hat{\mathbf{k}}) = \hat{k}_1^2\hat{k}_2^2\hat{k}_3^2. \tag{18}$$

The remaining (vectorial) functions have the components

$$G_\alpha(\hat{\mathbf{k}}) = 2s_2^2 - 3s_3(2s_2 - s_3)(1 - \hat{k}_\alpha^2), \qquad (\alpha = 1,2,3), \tag{19}$$

and

$$H_\alpha(\hat{\mathbf{k}}) = 2s_3^2 - 3s_2 s_3(2s_2 - s_3)\left[1 + \mathcal{P}(\hat{\mathbf{k}}) - \hat{k}_\alpha^2\right] \tag{20}$$

$$+ 9s_3^2(3s_2 - 2s_3)\hat{k}_\gamma^2\hat{k}_\delta^2, \qquad (\gamma \neq \delta, \quad \delta \neq \alpha). \tag{21}$$

The explicit expressions for $\tilde{c}(\hat{K})$ and $\tilde{v}_\alpha(\hat{K})$ read

$$\tilde{c}(\hat{K}) = \sqrt{1 + S(\hat{K})}, \qquad \tilde{v}_\alpha(\hat{K}) = [1 + S_\alpha(\hat{K})]\tilde{c}^{-1}(\hat{K})\hat{k}_\alpha, \tag{22}$$

where

$$S(\hat{K}) = 2\sqrt{G(\hat{\mathbf{k}})}\cos\left[\psi(\hat{\mathbf{k}}) + 2\pi j/3\right], \tag{23}$$

and

$$S_\alpha(\hat{K}) = \left[S(\hat{K})G_\alpha(\hat{\mathbf{k}}) + H_\alpha(\hat{\mathbf{k}})\right]/\left[S^2(\hat{K}) - G(\hat{\mathbf{k}})\right]. \tag{24}$$

For each j, the ratio of components of un-normalized polarization vectors $U_\alpha(\hat{K})$ (α=1, 2, 3) depends only on $C_3 = s_3/s_2$ (cf. [29])

$$U_1(\hat{K}) : U_2(\hat{K}) : U_3(\hat{K}) =$$

$$= \frac{\hat{k}_1}{T_j(\hat{\mathbf{k}}) - 3C_3\hat{k}_1} : \frac{\hat{k}_2}{T_j(\hat{\mathbf{k}}) - 3C_3\hat{k}_2} : \frac{\hat{k}_3}{T_j(\hat{\mathbf{k}}) - 3C_3\hat{k}_3}, \tag{25}$$

where

$$T_j(\hat{\mathbf{k}}) = 1 + G_0^{1/2}(\hat{\mathbf{k}})\cos[\psi(\hat{\mathbf{k}}) + 2\pi j/3], \quad (j = 0, 1, 2,). \tag{26}$$

Equations (14-26) are used for the calculation of the phase velocity and components of group velocity as well as the components of polarization vectors. The Every formulae should be used with caution for $\hat{\mathbf{k}}$ directed along high symmetry axes and for elastic constants obeying the conditions $s_3 = 0$ (isotropic media) and $s_2 = s_3$ (auxetics).

IV.3. Third-order elastic constants for isotropic and cubic media

For isotropic media tensor $\mathcal{C}_3$ depends on three parameters α, β and γ [27]

$$\begin{aligned} C_{\alpha_1\mu_1,\alpha_2\mu_2,\alpha_3\mu_3} &= \alpha\delta_{\alpha_1,\mu_1}\delta_{\alpha_2,\mu_2}\delta_{\alpha_3,\mu_3} + \beta[\delta_{\alpha_1,\mu_1}(\delta_{\alpha_2,\alpha_3}\delta_{\mu_2,\mu_3} + \delta_{\alpha_2,\mu_3}\delta_{\mu_2,\alpha_3}) + \\ &+ \delta_{\alpha_2,\mu_2}(\delta_{\alpha_1,\alpha_3}\delta_{\mu_1,\mu_3} + \delta_{\alpha_1,\mu_3}\delta_{\mu_1,\alpha_3}) + \delta_{\alpha_3,\mu_3}(\delta_{\alpha_1,\alpha_2}\delta_{\mu_1,\mu_2} + \delta_{\alpha_1,\mu_2}\delta_{\mu_1,\alpha_2})] + \\ &+ \gamma[\delta_{\mu_1,\mu_3}(\delta_{\alpha_1,\alpha_2}\delta_{\mu_2,\alpha_3} + \delta_{\alpha_1,\mu_2}\delta_{\alpha_2,\alpha_3}) + \delta_{\alpha_1,\mu_3}(\delta_{\mu_1,\alpha_2}\delta_{\mu_2,\alpha_3} + \delta_{\mu_1,\mu_2}\delta_{\alpha_2,\alpha_3}) + \\ &+ \delta_{\mu_1,\alpha_3}(\delta_{\alpha_1,\alpha_2}\delta_{\mu_2,\mu_3} + \delta_{\alpha_1,\mu_2}\delta_{\alpha_2,\mu_3}) + \delta_{\alpha_1,\alpha_3}(\delta_{\mu_1,\alpha_2}\delta_{\mu_2,\mu_3} + \delta_{\mu_1,\mu_2}\delta_{\alpha_2,\mu_3})]. \end{aligned} \tag{27}$$

For cubic media the following components of $\mathcal{C}_3$ do not vanish (cf. [23]): $\mathbf{C}_{111} = C_{222} = C_{333}$ $\mathbf{C}_{112} = C_{113} = C_{122} = C_{133} = C_{223} = C_{233}$; $\mathbf{C}_{123}$; $\mathbf{C}_{144} = C_{255} = C_{366}$; $C_{155} = \mathbf{C}_{166} = C_{244} = C_{266} = C_{344} = C_{355}$ and $\mathbf{C}_{456}$. Thus, there are six independent components of $\mathcal{C}_3$, which depend on α, β and γ.

Using Fedorov's method mentioned in Sect. IV.1.1, Tamura introduced the third order elastic constants for the effective isotropic system. Using a different method we calculated them for all crystal classes [25],

IV.4. Characteristics of long wavelength acoustic phonons

Consider an anisotropic crystalline medium. For small wave vectors ($ka \ll 1$), $k = |\mathbf{k}|$, where a is the lattice constant, i.e. for long wave-length acoustic phonons, the frequency is linear in the magnitude k of the wave vector $\mathbf{k}$

$$\omega = 2\pi\nu = c(\hat{\mathbf{k}}, j)k.$$

The phase velocity $c(\hat{\mathbf{k}}, j)$ depends only on the polarization j ($j = 0$ for quasi-longitudinal, $j = 1$ for fast quasi-transverse and $j = 2$ for slow quasi-transverse phonons) and on the direction $\hat{\mathbf{k}}$ of the wave vector $\mathbf{k}$ (or on polar ϕ_k and azimuthal θ_k angles). Thus phonons are characterized by the set $(k, \hat{K})$ or by $(\nu, \hat{K})$

Consider the mean value of a function A of $(\hat{K}) \equiv (\hat{\mathbf{k}}, j)$

$$\left\langle A(\hat{K}) \right\rangle = \frac{1}{3} \sum_{j=0}^{2} \int_{4\pi} \frac{\mathrm{d}\hat{k}}{4\pi} A(\hat{K}) . \tag{28}$$

The Debye velocity c_D is defined in terms of mean value of $c^{-3}(\hat{K})$

$$C_D^{-3} = \left\langle c^{-3}(\hat{K}) \right\rangle_{\hat{K}} = c^{-3} \left\langle \tilde{c}^{-3}(\hat{K}) \right\rangle_{\hat{K}} . \tag{29}$$

Isotropic media are characterized by two constant velocities c_l and c_t hence Eq. (29) gives

$$\frac{1}{c_D^3} = \frac{2}{c_t^3} + \frac{1}{c_l^3} . \tag{30}$$

In [8] (cf. also [17]) we considered the slowness surface of phonons $\hat{K}$. It is defined by the vector equation

$$\mathbf{k}_j = s(\hat{K}) \hat{\mathbf{k}} , \tag{31}$$

where the slowness $s(\hat{K}) \equiv c^{-1}(\hat{K})$

Generally we shall study spatially inhomogeneous non-equilibrium states of phonon gases, so a phonon is a wave packet carrying the energy $w = \hbar\omega$ and the quasi-momentum $\tilde{\mathbf{p}} = \hbar\mathbf{k}$. It moves with the group velocity

$$\mathbf{v}(K) = \vec{\nabla}_k \omega(K) . \tag{32}$$

For long wave-length acoustic phonons the group velocity depends only on $\hat{K}$ and s_2, s_3 *via* functions introduced in Sect. IV.2.2. As a rale, the group velocity vector is not parallel to the wave vector, so it is an anisotropic quantity. Only for isotropic media $\mathbf{v}(\hat{K}) = c_\sigma \hat{\mathbf{k}}$. ($\sigma = l, t$). For anisotropic media and for each direction of $\mathbf{k}$ phase velocity does not exceed group velocity [24]

$$\mathbf{v}(\hat{K}) \hat{\mathbf{k}} = c(\hat{K}) . \tag{33}$$

V. SCATTERING OF LONG WAVELENGTH ACOUSTIC PHONONS BY POINT MASS DEFECTS

In this section we assume that the down-conversion processes are very rare, so the elastic scattering processes dominate. Consider a crystalline dielectric or semiconducting specimen of volume V with fluctuations in the mass distribution. Suppose that these fluctuations arise from

the presence of PMDs and that the crystalline lattice contains no other lattice defects. We assume that the specimen contains N elementary cells and that the volume of each is v_0.

V.1. The Boltzmann kinetic equation

Consider a rarefied gas of LAPs. A non-equilibrium state of this gas is characterized by the distribution function f. This function depends on time t, spatial variables $\mathbf{r} = (x, y, z)$, phonon frequency ω, the direction $\hat{\mathbf{k}}$ of the wave vector and on the polarization j. Since in the case of scattering of phonons by PMDs only $\hat{K}$ may change, we will further restrict ourselves to phonons of a given frequency and omit the dummy parameter ω.

Assume that the unit cell of our crystal contains r atoms which are enumerated by the index σ. Suppose further that a σ-th atom can be substituted by isotope atoms enumerated by the index i ($i = 1,2, ...,p$) of the masses $M^i_\sigma = A^i_\sigma M_{amu}$, where A^i_σ is the mass number and M_{amu} is the atomic mass unit. The corresponding abundance is f^i_σ. Thus, the average mass of the σ-type atom is

$$\bar{M}_\sigma = \sum_{i=1}^{p} f^i_\sigma M^i_\sigma = \sum_{i=1}^{p} f^i_\sigma A^i_\sigma M_{amu} \equiv \bar{A}_\sigma M_{amu}. \tag{34}$$

The simplest characteristics of the scattering processes is the mean free time τ- the average time elapsing between successive collisions (here - the Rayleigh time). The inverse of this quantity is proportional to the factor $\tilde{g}$ [30,31]

$$\tau^{-1} \equiv \tau^{-1}(\omega) = \frac{v_0 \tilde{g} \omega^4}{4\pi c_D^3} = 4\pi^3 \frac{v_0 \tilde{g} \nu^4}{c_D^3} \equiv \alpha_{sc} \nu^4, \tag{35}$$

where ν is the linear frequency and

$$\tilde{g} = \frac{\sum_{\sigma=1}^{r} g_\sigma [\bar{A}_\sigma]^2}{\sum_{\sigma=1}^{r} [\bar{A}_\sigma]^2}. \tag{36}$$

The coefficient g_σ is defined as

$$g_\sigma = \sum_{i=1}^{p} f^i_\sigma \left(1 - \frac{A^i_\sigma}{\bar{A}_\sigma}\right)^2. \tag{37}$$

For Bravais lattices containing one (host) atom in the elementary cell and one kind of isotope (substitutional) atoms ($\sigma = 1$, $i = 1$) with the atomic mass numbers respectively A_h, A_i

$$\tilde{g} = g_{imp} \equiv c_{imp} \left(\frac{A_h}{A_i} - 1\right)^2, \tag{38}$$

where c_{imp} is the concentration of isotope (substitutional) atoms.

In the kinetic regime phonon distribution function obeys the Boltzmann equation

$$\frac{\partial f(K;\mathbf{r},t)}{\partial t} + \mathbf{v}(K)\nabla f(K;\mathbf{r},t) = \left[\frac{\mathrm{d}f(K;\mathbf{r},t)}{\mathrm{d}t}\right]_{coll}. \tag{39}$$

Generally, scattering and anharmonic processes are characterized by a non-vanishing rate of change $[df/dt]_{coll}$. The contribution $[df/dt]_{PMD}$ of elastic scattering to the $[df/dt]_{coll}$ term contains one term which is a *linear functional* of the distribution function, namely

$$\left[\frac{\mathrm{d}f}{\mathrm{d}t}\right]_{PMD} \equiv \mathbf{B}f(K;\mathbf{r},t) =$$
$$= \frac{V}{(2\pi)^3}\sum_{j=0}^{2}\int \mathrm{d}^3k' w(K,K')[f(K';\mathbf{r},t) - f(K;\mathbf{r},t)]. \tag{40}$$

The kernel of this integral functional is the probability density of transitions per unit time (transition rates), which for Bravais lattices is equal to

$$w(K,K') \equiv w(K',K) =$$
$$= \frac{\pi}{2N}\tilde{g}\,\omega(K)\,\omega(K') \times |\mathbf{e}(\hat{K})\,\mathbf{e}(\hat{K}')|^2\,\delta[\omega(K) - \omega(K')]. \tag{41}$$

For LAPs the collision integral $[df/dt]_{PMD}$ can be written in a different form

$$\mathbf{B}f(\hat{K};\mathbf{r},t) = -\tau^{-1}\nu(\hat{K})f(\hat{K};\mathbf{r},t) + 3\tau^{-1}\mathcal{E}_{\alpha\beta}(\hat{K})\left\langle \mathcal{E}_{\alpha\beta}(\hat{K}')f(\hat{K}';\mathbf{r},t)\right\rangle_{\hat{K}'}, \tag{42}$$

where

$$\nu(\hat{K}) \equiv 3\,\mathcal{E}_{\alpha\beta}(\hat{K})\left\langle \mathcal{E}_{\alpha\beta}(\hat{K}')\right\rangle_{K'},$$

and $\mathcal{E}_{\alpha\beta}(\hat{K})$ is an element of the *dyad* $\mathcal{E}^{(2)}$

$$(\mathcal{E}^{(2)})_{\alpha\beta} \equiv \mathcal{E}_{\alpha\beta} \equiv [\mathbf{e}(\hat{K}) \otimes \mathbf{e}(\hat{K})]_{\alpha\beta} = e_\alpha(\hat{K})\,e_\beta(\hat{K}). \tag{43}$$

Further we shall employ abbreviated notation $\mathbf{e} = \mathbf{e}(\hat{K})$, $\mathbf{e}' = \mathbf{e}(\hat{K}')$, etc.

As we know, for long wavelength acoustic phonons a crystalline solid can be considered as an anisotropic continuous elastic medium. Therefore, the problem of calculating the polarization vectors and frequencies is relatively simple and model independent (cf. [24,29]). Knowing them one can establish the spectrum of relaxation rates (i.e. the spectrum of the operator **B)** (cf. [13]).

One can show that the solution of the Boltzmann equation (39), without the collision term and supplemented with a quite general term describing the phonon generation, yields strongly

anisotropic densities of currents of energy and quasi-momentum and allows to account for the phenomenon of focusing (cf. [13, 32]). Therefore, generally, the kinetic equation provides the general method of accounting for generation, propagation, scattering and decay processes of phonons. However, even in the simplest case of scattering by point mass defects embedded in an isotropic medium in the absence of down-conversion processes the explicit formulae for time and space dependent densities are not known. Therefore, one ought to relay on the results of computer experiments.

V.l.l. Scattering rates for isotropic media

For isotropic media any pair of mutually orthogonal unit vectors which are pexpendicular to the wave vector k provides the polarization vectors of transverse modes (j = 1,2). Therefore, the calculation of scattering rates needs some accuracy.

Consider a triple of polarization vectors of incoming phonons $\mathbf{e}_{t1}$, $\mathbf{e}_{t2}$, $\mathbf{e}_l = \hat{\mathbf{k}}$. A triple of outgoing polarization vectors $\mathbf{e}_{t1}'$, $\mathbf{e}_{t2}'$, $\mathbf{e}_l' = \hat{\mathbf{k}}'$, can be obtained by rotation by the Euler angles $\vartheta, \varphi, \psi (-\pi \le \vartheta \le \pi, 0 \le \varphi, \psi \le 2\pi$ [33].

$$\begin{Bmatrix} \mathbf{e}_l'(\vartheta, \varphi, \psi) \\ \mathbf{e}_{t_1}'(\vartheta, \varphi, \psi) \\ \mathbf{e}_{t_2}'(\vartheta, \varphi, \psi) \end{Bmatrix} = \begin{Bmatrix} a_{ll}(\vartheta, \varphi, \psi) & a_{ll_1}(\vartheta, \varphi, \psi) & a_{ll_2}(\vartheta, \varphi, \psi) \\ a_{t_1 l}(\vartheta, \varphi, \psi) & a_{t_1 t_1}(\vartheta, \varphi, \psi) & a_{t_1 t_2}(\vartheta, \varphi, \psi) \\ a_{t_2 l}(\vartheta, \varphi, \psi) & a_{t_2 t_1}(\vartheta, \varphi, \psi) & a_{t_2 t_2}(\vartheta, \varphi, \psi) \end{Bmatrix} \begin{Bmatrix} \mathbf{e}_l(\hat{\mathbf{k}}) \\ \mathbf{e}_{t_1}(\hat{\mathbf{k}}) \\ \mathbf{e}_{t_2}(\hat{\mathbf{k}}) \end{Bmatrix}$$

Coefficients $a_{jj'}$ $(j, j' = l, t_1, t_2)$ are given by Goldstein [33]. Introduce an orthogonal matrix $\mathbf{A}$ with elements $a_{j'j}$. Since $\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}_2$ the vectors $\mathbf{e}'$ are orthonormal. Similarly, since $\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}_2$ these vectors comprise a complete set.

Relative orientation of pairs $(\mathbf{e}_{t1}, \mathbf{e}_{t2})$ and $(\mathbf{e}_{t1}', \mathbf{e}_{t2}')$ depends only on the angle ψ. Since all different relative orientations of them are of the same importance, we should account for all of them, i.e. average the probability densities over the angle ψ. By calculating scalar products $\mathbf{e}_j, \mathbf{e}_{j'}$. $(j,.j' = l, t_1, t_2)$ and averaging them, we obtain the normalized transition rates

$$w_{j \to j'}(\vartheta, \varphi) = \Lambda_j \int_0^{2\pi} \frac{\mathrm{d}\psi}{2\pi} a_{j'j}^2(\hat{\mathbf{k}}, \psi; \vartheta, \varphi), \qquad (j, j' = l, t_1, t_2), \tag{44}$$

where

$$\Lambda_j = \frac{1}{\tau(\omega)} \left(\frac{c_D}{c_j} \right)^3 .$$

With the help of Eq. (4.46) of [33] we obtain

$$
\begin{aligned}
&w_{t_1\to t_1} = w_{t_1\to t_2} = \frac{1}{2}\Lambda_t[\cos^2\varphi + \cos^2\vartheta\sin^2\varphi],\\
&w_{t_1\to l} = \Lambda_l\sin^2\vartheta\sin^2\varphi, \quad w_{t_2\to l} = \Lambda_l\sin^2\vartheta\cos^2\varphi,\\
&w_{t_2\to t_1} = w_{t_2\to t_2} = \frac{1}{2}\Lambda_t[\sin^2\varphi + \cos^2\vartheta\cos^2\varphi],\\
&w_{l\to t_1} = w_{l\to t_2} = \frac{1}{2}\Lambda_t\sin^2\vartheta, \qquad w_{l\to l} = \Lambda_l^2\cos^2\vartheta.
\end{aligned}
\tag{45}
$$

For each j the transition probabilities obey the identity

$$
\frac{1}{4\pi}\sum_{j'=t_1,t_2,l}\int_0^{2\pi}\mathrm{d}\varphi\int_{-\pi}^{\pi}\mathrm{d}\vartheta\sin\vartheta\, w_{jj'}(\vartheta,\varphi) = \frac{1}{3\tau(\omega)}, \qquad (j = l, t_1, t_2). \tag{46}
$$

Adding Eqs. (45) we obtain

$$
\begin{aligned}
w_{T\to T} &= \Lambda_t[1 + \cos^2\vartheta]\\
w_{T\to L} &= \Lambda_l[1 - \cos^2\vartheta]\\
w_{L\to T} &= \Lambda_t[1 - \cos^2\vartheta].
\end{aligned}
\tag{47}
$$

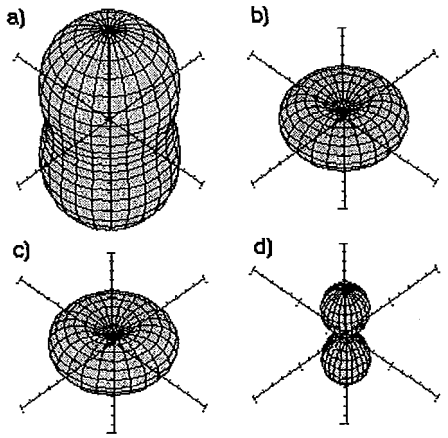

Fig. 1. The dependence on angles of probabilities of scattering of phonons by point mass defects embedded in isotropic medium as a function of outgoing phonon direction. The direction of incoming phonon is fixed. (a) $T \to T$; (b) $T \to L$; (c) $L \to T$; (d) $L \to L$

Plots of angular dependencies of the transition probabilities (47) are shown in Figs. la-d. The expressions (47) are used in our simulations of propagation and scattering of down-converting phonons in isotropic media.

V.2. Long-time asymptotics of the distribution function

Suppose that an injected pulse of phonons propagate in an elastic medium and scatters on point mass defects. After lapses of time much longer than the Rayleigh time $\tau(\omega)$ phonons are registered by a detector which *absorbs* them. Studying the long-time asymptotics of the Fourier-Laplace transform of the distribution function $f(\omega, \hat{K}; \mathbf{r}, t)$ or using the Chapman-Enskog approach, we derived the diffusion equation (cf. [13]) from the Boltzmann equation. The density of phonons of a given frequency

$$N(\omega; \mathbf{r}, t) = \left\langle f(\omega, \hat{K}; \mathbf{r}, t) \right\rangle_{\hat{K}} \tag{48}$$

fulfills the diffusion equation

$$\frac{\partial N(\omega, \mathbf{r}, t)}{\partial t} = D_{\alpha\beta} \frac{\partial^2}{\partial r_\alpha \partial r_\beta} N(\omega; \mathbf{r}, t) . \tag{49}$$

We obtained a general formula for the elements of the matrix $\mathcal{D}$ of diffusion coefficients $D_{\alpha\beta}$ valid for a medium of arbitrary symmetry [13]. For isotropic and cubic media the matrix $\mathcal{D}$ is proportional to the unit matrix

$$D_{\alpha\beta}(\omega) = D(\omega)\, \delta_{\alpha,\beta} . \tag{50}$$

For both isotropic and cubic media we have obtained (cf. [9, 12])

$$D = \frac{1}{3} \tau \left\langle v^2(\hat{K}) \right\rangle_{\hat{K}} . \tag{51}$$

The coefficient $\tau(35)$ depends on the experimental conditions, but the last factor of Eq. (51) is universal. Its values, for different cubic materials, are collected in a table enclosed within our paper [12].

Each computer experiment on the diffusive propagation of phonons should be performed for a given geometry. Therefore, we should obtain solutions of the diffusion equation for the corresponding choice of the geometrical form of specimen and of the boundary as well as the initial conditions. We consider here diffusion in a sphere.

V.3. Diffusion in a sphere

Suppose that phonons propagate diffusively in a sphere of the radius R. The solution of the diffusion equation (49) obeying the following boundary and initial conditions

$$N(\mathbf{r} = \hat{\mathbf{r}} R, t) = 0 , \tag{52}$$

$$N(\mathbf{r}, t = 0) = N_v \delta(\mathbf{r}) \equiv N_v \frac{\delta(r)}{2\pi r^2} , \tag{53}$$

depends only on the length r of the vector $\mathbf{r}$ and can be obtained from the solution derived in [34]

$$N(r, t) = N_v \theta(R - r) \frac{1}{R^2 r} \sum_{n=1}^{\infty} \exp\left[-\left(\frac{\pi n}{R} \right)^2 Dt \right] n \sin\left(\frac{n\pi}{R} r \right) . \tag{54}$$

The flux density of phonons at frequency ω through the unit sphere at time t looks like (cf. [34])

$$j(t) = N_v \sum_{n=1}^{\infty} (-1)^n n^2 \exp[-\pi^2 n^2 Dt], \qquad (r = R = 1). \tag{55}$$

This quantity is measured in our computer experiments on the diffusive propagation of phonon beams (cf. Sect. VIII.3.2).

The function $j(t)$ depends only on $x = \sqrt{Dt}$ and attains the maximum value $j_{max} = 0.300015$ at $x_{max} = 0.30291$, and has two inflection points: one on the front part of the diffusive pulse at $x_{fi} = 0.21275$ ($j_{fi} = 0.118931$) and the second on the tail part at $x_{ti} = 0.37427$ ($j_{ti} = 0.235123$). These three points are used by Ivanov et al for characterizing the diffusive pulses [35],

The normalization condition for $j(t)$ reads

$$4\pi \int_0^{\infty} \mathrm{d}t j(t) = N_v,$$

where N_v is the initial number of phonons injected to the specimen by the source. From the normalization condition it follows that the flux density scales with $D^{-1} \sim \tilde{g} \sim \alpha_{sc}$ whereas $x^2_{max}, x_{fi}^2, x_{ti}^2$ scales with $D \sim \tilde{g}^{-1} \sim \alpha_{sc}^{-1}$.

V.4. Down-conversion processes in isotropic media

According to Eq. (20) of [8] (cf. also [17]) the tensor of second order elastic constants $\mathcal{C}_2$ with components $C_{\alpha\mu,\ \beta\nu}$ defines the dispersion-less frequencies $\omega(K) = c(\hat{K})k$. In the frame of elasticity theory the tensor of third order elastic constants $\mathcal{C}_3$ with elements $C_{\alpha 1\mu 1, \alpha 2\mu 2, \alpha 3\mu 3}$ together with elements of $\mathcal{C}_2$, defines the probability density of three-phonon anharmonic processes [36],

Consider an acoustic phonon $K = (\mathbf{k}, j)$ with the energy $w = \hbar\omega$ and quasi-momentum $\vec{p} = \hbar\mathbf{k}$, in an isotropic nonlinear elastic medium. The degenerate transverse acoustic phonons *(TA)* with the phase velocity $c_t^{(ef)}$ (13) are stable against spontaneous down-conversion processes. However, in agreement with the conservation of energy and quasi-momentum laws only longitudinal acoustic phonons with the phase velocity $c_l^{(ef)}$ (13) can split. Polarizations of the daughter phonons obey some selection rules [37, 38], There are three possible splitting processes of *LA* phonons, namely: (I) $LA \to LA + TA$, (II) $LA \to TA + TA$ and (III) $LA \to LA + LA$ [361. The second process dominates, whereas the third one gives the smallest contribution to the relaxation rate of *LA* phonons. Tamura [37] a calculated the suitable matrix elements and relaxation rates.

For isotropic media matrix elements $M(K; K', K'')$ corresponding to processes (I)-(III) depend only on Lamé's parameters λ and μ (cf. Sect. IV. 1.1) and on β and γ-two of three parameters which characterize the third order elastic constants (cf. Sect. IV.3). The above matrix elements depend also on the angle between $\mathbf{k}$ and $\mathbf{k}'$. In the process (I) a daughter *TA* phonon is polarized perpendicularly to the plane *II* spanned by vectors $\hat{\mathbf{k}}, \hat{\mathbf{k}}'$ and

$$M_{\mathrm{I}}(\mathbf{k}; \mathbf{k}'\mathbf{k}'') = \frac{1}{2}(2\beta + 4\gamma + \lambda + 3\mu)\frac{kk'}{k''}\left[k^2 - (k')^2\right]\sin(2\theta). \tag{56}$$

For process (II) the final *TA* phonons can be IIa) simultaneously polarized *in II*, or (IIb) simultaneously polarized *perpendicularly* to *II*. The corresponding matrix elements are

$$M_{IIa}(\mathbf{k};\mathbf{k}'\mathbf{k}'') = \frac{kk'}{k''}\{[\beta + \lambda + (2\gamma + \mu)](k' - k\cos\theta)^2 + \\ - (\beta + 2\gamma + \mu)k^2\sin^2\theta\}, \tag{57}$$

$$M_{IIb}(\mathbf{k};\mathbf{k}'\mathbf{k}'') = kk'[(\beta + \lambda)(k\cos\theta - k') + 2(\gamma + \mu)(k - k'\cos\theta)\cos\theta]. \tag{58}$$

In our calculations we use formulae (56-58) and account for the conservation laws

$$c_l k = c_\sigma k' + c_t k'', \qquad (\sigma = l, t), \tag{59}$$

$$\mathbf{k} = \mathbf{k}' + \mathbf{k}''. \tag{60}$$

Because the wave number k is very small we can omit the Umklapp processes. For process (III) from the conservation laws it follows that the vectors $\mathbf{k}$, $\mathbf{k}'$, $\mathbf{k}''$ are collinear, so the corresponding volume of the k-space is very small, and thus the related relaxation rate is negligible.

Having calculated the matrix elements we can find the relaxation rates for anharmonic phonon processes [37]

$$\tau^{-1}_{L\to L+T} = \frac{\hbar\omega^5}{256\pi\rho^3}\frac{\delta^2 - 1}{c_l^9}(2\beta + 4\gamma + \lambda + 3\mu)^2 I_{L\to L+T}(\xi_0) = \alpha_{L\to L+T}v^5, \tag{61}$$

where

$$\alpha_{L\to L+T} = \left(\frac{h\pi^3}{16\rho^3}\right)\frac{\delta^2 - 1}{c_l^9}(2\beta + 4\gamma + \lambda + 3\mu)^2 I_{L\to L+T}(\xi_0). \tag{62}$$

The coefficients λ and μ present in formulae (61) are the Lamé coefficients (12). Similarly

$$I_{L\to L+T}(\xi_0) = \int_{\xi_0}^{1}\frac{\mathrm{d}\xi}{\xi^2}(1 - \xi^2)^2\left[(1 + \xi)^2 - \delta^2(1 - \xi)^2\right]\times \\ \times\left[1 + \xi^2 - \delta^2(1 - \xi)^2\right]^2, \tag{63}$$

and

$$\tau^{-1}_{L\to T+T} = \frac{\hbar\omega^5}{32\pi\rho^3}\frac{1}{(c_l^2 c_t)^3} I_{L\to T+T}(\xi_1, \xi_2) \equiv \alpha_{L\to T+T}v^5, \tag{64}$$

where

$$I_{L\to T+T}(\xi_1,\xi_2)=\int_{\xi_1}^{\xi_2}\mathrm{d}\xi\left\{\left(A+B\delta\xi-B\xi^2\right)^2+\right.$$
$$\left.+\left[C\xi(\delta-\xi)-\frac{D}{\delta-\xi}\left(\xi-\delta-\frac{1-\delta^2}{4\xi}\right)\right]^2\right\}, \tag{65}$$

while

$$A=\frac{1}{2}(1-\delta^2)[\beta+\lambda+(1+\delta^2)(\gamma+\mu)],\quad B=[\beta+\lambda+2\delta^2(\gamma+\mu)],$$
$$C=[\beta+\lambda+2(\gamma+\mu)],\qquad D=(1-\delta^2)(2\beta+4\gamma+\lambda+3\mu), \tag{66}$$
$$\delta=(c_l/c_t)^2=(\lambda+2\mu)/\mu,\qquad \xi_0=\frac{\delta-1}{\delta+1},\qquad \xi_1=\frac{\delta-1}{2},\qquad \xi_2=\frac{\delta+1}{2},$$

and

$$\alpha_{L\to T+T}=\frac{h\pi^3}{2\rho^3}\frac{1}{(c_l^2c_t)^3}I_{L\to T+T}(\xi_1,\xi_2). \tag{67}$$

To derive explicit expressions for third order elastic constants for an equivalent isotropic medium Tamura [37] a used Fedorov's approach [24] (which was proposed for second order elastic constants). The method used in Sect. IV. 1.1 yields the same results [25]

$$\alpha_{eff}=\frac{1}{35}(C_{111}+18C_{112}+16C_{123}-30C_{144}-12C_{166}+16C_{456}),$$
$$\beta_{eff}=\frac{1}{35}(C_{111}+4C_{112}-5C_{123}+19C_{144}+2C_{166}-12C_{456}), \tag{68}$$
$$\gamma_{eff}=\frac{1}{35}(C_{111}-3C_{112}+2C_{123}-9C_{144}+9C_{166}+9C_{456}).$$

Formulae (61-68) are used in the program for calculation of the probabilities of down-conversion processes in the effective isotropic medium corresponding to the chosen cubic medium.

VI. THE SIMULATION ALGORITHM

VI. 1. General remarks

We may divide each step of simulation of the propagation a phonon in a non-ideal crystalline medium into several steps which are processed in the loop. Each step consists of:

- The choice of the duration of a free flight interval between successive scattering or down conversion events. If a phonon leaves the sample the propagation is interrupted.
- The choice of the kind of event which terminates the pending step of free flight.
- Determination of the characteristics of an outgoing phonon (phonons).

Between the successive scattering or conversion events a phonon moves along a straight line with the corresponding group velocity $\mathbf{v}_g(\hat{\mathbf{k}}, j)$. The duration of the free flight for each step of propagation is chosen at random.

Next, one should choose the kind of the act terminating an event of free motion - it can be a scattering or a down conversion event. In the former case characteristics of an outgoing phonon, in the latter one - characteristics of two daughter phonons should be randomly chosen. The suitable probability densities should account for: (i) characteristics of an incoming phonon, (ii) the conservation laws of energy and quasi-momentum, and (iii) density of final phonon states. If a down conversion event is drown up one should choose a particular realization of it.

Since we are using Monte Carlo method the important problem in our simulations is random selection of the numbers from a finite interval with a given density of probability.

VI.2. Generation of random numbers

A typical random number generator produces the numbers from the interval [0, 1) with a uniform density. In fact one frequently needs random numbers which belong to other intervals (or even to subspaces of greater dimensionality than 1) and distributed with other densities than the uniform one. The change of the interval [0, 1) to [a, b) can be done with a simple linear transformation $y' = a + (b - a)y$, where $y \in [0, 1)$. The methods of obtaining the desired distribution are more complicated.

We used two methods for the generation of random numbers, namely the direct and the rejection techniques. Since they were described by Jacoboni and Reggiani [39], we describe them very briefly. Both techniques can be used for bounded probability density function $p(y)$ and a finite interval [a, b).

VI.2.1. The direct technique

Assume that function $p(y)$ is defined on the interval [a, b). Introduce the recalculating function $f(u)$ defined as

$$f^{-1}(u) = \frac{\int_a^u dy\, p(y)}{\int_a^b dy\, p(y)}. \tag{69}$$

The formula $y = f(a + (b - a)u)$ allows one to generate random numbers y distributed between a and b with distribution $p(y)$, when $x \in [0,1)$ has uniform distribution. We used this method for the random choice of directions of phonon wave vectors of in both this and previous program [8], Namely for the polar angle $\phi_k \in (0, 2\pi)$ we use the uniform distribution, the azimuthal angle $\theta_k \in (-\pi/2, \pi/2)$ is calculated with

$$p(y) = \arcsin(2y - 1).$$

VI.2.2. The rejection technique

When for given function *p(y)* the function $f(u)$ (defined by Eq. (69)) does not exist, one should use a more time consuming techniques. The most simple method is called rejection technique.

Let C be a positive number such that $C \geq f(x) > 0$ in the whole $[a, b)$ and y_i, y_i' are two random numbers obtained with a flat distribution function in $[a, b)$ and [0, C), respectively.

In the process of generation of random numbers we reject all pairs y_i, y_i'- if the condition $y_i' \leq p(y_i)$ is violated. When this condition is satisfied, the returned number y_i- is one of random numbers distributed with density *p(y)*.

VI.3. Random choice of the interval of ballistic motion and of an event terminating it

The expressions for the probability densities per unit time interval of elastic scattering (Eq. (41)) and of down conversion processes (Eqs. (56-59)) are used for making the random choice of the duration time of a free flight event. For this purpose we use in the interval $[0, \infty)$ such exponential distribution function which for the mean value of the inverse of free flight duration $\langle t^{-1} \rangle$ gives

$$\left\langle t^{-1} \right\rangle = \tau_R^{-1} \equiv \begin{cases} \dfrac{1}{\tau_{scat}} & \text{for } FT \text{ and } ST, \\ \left[\dfrac{1}{\tau_{scat}} + \dfrac{1}{\tau_{L \to L+T}} + \dfrac{1}{\tau_{L \to T+T}} \right] & \text{for L.} \end{cases} \tag{70}$$

Since the durations of free flights is distributed exponentially

$$p(t) = \frac{1}{\tau_R} \exp\left(-\frac{t}{\tau_R} \right),$$

one can use the direct method of generation with recalculating function of the following form

$$t^{-1} = -\left\langle t^{-1} \right\rangle \ln y = -\tau_R^{-1} \ln y, \tag{71}$$

where *y* is a pseudo-random number belonging to the interval [0, 1).

In fact according to Eqs. (35, 56-58) and Table I the only phonon characteristic entering expressions for characteristic times τ_s $(s = scat, L \to L + T, L \to T + T)$ is the frequency *v*, thus in agreement with Eqs. (35), (61) and (65).

$$\tau_{scat}^{-1} = \alpha_{scat} v^4, \quad \tau_{L \to L+T}^{-1} = \alpha_{L \to L+T} v^5, \quad \tau_{L \to T+T}^{-1} = \alpha_{L \to T+T} v^5. \tag{72}$$

Coefficients α_s $(s = scat, L \to L + T, L \to T + T)$ depend on elastic characteristics of media, α_{scat} depends additionally on characteristics of scatterers.

For longitudinal phonons we define the probability of the event of the type s as the ratio $p_s \equiv \tau_s/\tau_R$ ($p_s \in [0, 1)$, $\Sigma_s p_s = 1$). In isotropic media down conversion of transverse phonons is forbidden.

VI A Scattering on point mass defects

In agreement with Eq. (41) we introduce p_{dir} - the un-normalized probability density of scattering transforming an incoming phonon $(\hat{\mathbf{k}}, j)$ into a phonon $(\hat{\mathbf{k}}', j')$

$$p_{dir}(\hat{\mathbf{k}}, j, \hat{\mathbf{k}}', j') = \left[\frac{c_{\max}}{c(\hat{\mathbf{k}}', j')}\right]^3 |\vec{e}(\hat{\mathbf{k}}, j)\,\vec{e}(\hat{\mathbf{k}}', j')|^2, \tag{73}$$

where $c_{\max}$ is the maximal value of phase velocity

$$c_{\max} = \sup_{\substack{\hat{\mathbf{k}} \in 4\pi \\ j = L, ST, FT}} c(\hat{\mathbf{k}}, j).$$

Since $0 \le p_{dir} \le 1$ this probability distribution can be directly used for generation of random numbers using the rejection technique. This method is rather slow (approximately 20 rejection events per one random point), but we are not able to find recalculation function for this problem.

According Sect. V. 1. in the case of an isotropic medium the scattering probability densities depend only on one angle υ between the polarization vectors of the incoming and outgoing phonon. Here we can use the direct method.

VI.5. **Phonon down-conversion processes**

VI. 5.1. Anisotropic media

Generally the density probability of down-conversion processes depends on three wave vectors, i.e. on nine parameters. Since the wave vector of an incoming phonon is given, one has to operate with the set

$$\bigotimes_{i=1}^{2} R_i^3 \otimes P$$

where P is the discrete set of all pairs of polarization indices. Using the quasi-momentum conservation law we can eliminate three parameters. Unfortunately, because the phase velocities are rather complicated functions of directions of wave vectors the energy conservation law cannot be used for further reduction of the number of independent parameters.

Since phonons involved in down conversion processes have finite life-time τ_{ph} their energies are defined with the accuracy $\epsilon \approx \hbar\Delta\omega \sim \hbar/\tau_{ph}$ (where $\Delta\omega \ll \omega_i$). Hence, the energy conservation law $\omega_i - \omega_f^{(1)} - \omega_f^{(2)} = 0$ should be modified

$$\hbar(\omega_i - \omega_f^{(1)} - \omega_f^{(2)}) \approx \epsilon.$$

However, in such case the time cost of random selection (the number of rejection per one accepted random point) of a pair of outgoing phonons is rather high, being proportional to ϵ^{-1}.

VI.5.2. Down-conversion processes in an isotropic medium

In an isotropic medium all three wave vectors of phonons taking part in a down-conversion event, namely the vectors $\hat{\mathbf{k}}_i$, $\hat{\mathbf{k}}_f^{(1)}$ and $\hat{\mathbf{k}}_f^{(2)}$, lay in a plane called the reaction plane. Due to symmetry of isotropic media all reaction planes are equivalent, so one can consider all down-conversion processes in a plane using as the only free parameter of process the angle υ between wave vectors of the outgoing phonons. The angle φ defining the orientation of the particular reaction plane is selected at random with the uniform distribution function. The probability distribution function of υ as well as the interval of allowed angles (υ_1, υ_2) depend on the type of down-conversion process described in Sect. V.4. To choose the angle υ we are using in the program the rejection technique.

For the reaction channel $LA \rightarrow LA + TA$ one can use the direct method of generation of random numbers, and for process $LA \rightarrow TA + TA$ the recalculating function is unknown, so we used the rejection method. The generating procedures have been adapted from the Monte Carlo program of Kiev group [34],

VI. 5.3. The compromise: anisotropic propagation and scattering, isotropic down-conversion processes

Suppose that an incoming phonon $(\hat{\mathbf{k}}_i, j_i, \omega_i)$ propagating in a cubic medium down-converts to a pair of daughter (outgoing) phonons $(\hat{\mathbf{k}}_f^{(1)}, j_f^{(1)}, \omega_f^{(1)})$, $(\hat{\mathbf{k}}_f^{(2)}, j_f^{(2)}, \omega_f^{(2)})$. The characteristic of the *incoming* phonon are calculated with the help of formulae valid for *cubic* media. Since in our computer experiments processes of down-conversion happen in an *equivalent isotropic medium* the characteristic of *outgoing* phonons are calculated using equations valid for *isotropic* media. The angles φ and θ are randomly chosen. Knowing the angle φ for this value of θ with the help of the quasi-momentum conservation law one can calculate wave vectors of outgoing phonons. Their phase velocities are calculated with the help of formulae valid for cubic media. The lengths of wave vectors are scaled until the energy conservation law is fulfilled.

Since we discard colinear $LA \rightarrow LA + LA$ processes at last one of two outgoing phonons ought to be polarized transversely. According to the conservation laws it should be a FT phonon. So the ambiguity with the choice of kind of outgoing transverse phonons arises only for $LA \rightarrow TA + TA$ process. For them we choose the kind of outgoing transverse phonons using following probability densities

$$p(\hat{\mathbf{k}}, \sigma) = \frac{c^3(\hat{\mathbf{k}}, \sigma)}{\sum_{\gamma} c^3(\hat{\mathbf{k}}, \gamma)} \quad (\sigma, \gamma = FT, ST).$$

They are related to the corresponding densities of states $d(\hat{K}) = [c(\hat{K})/c_D]^3$.

VI. 5.4. Random choice of energies of phonons compatible with the Planckian distribution function

Consider the distribution function of energies of radiated phonons for the Planckian source of the temperature T

$$p'(\nu) = \frac{\nu^2}{\exp\left(\frac{h\nu}{k_B T}\right) - 1}. \tag{74}$$

In Monte Carlo experiments the random choice of energies of generated phonons should reproduce $p'(\nu)$.

Since for any integration interval $[0, \nu)$ $(\nu < \infty)$ the integral of $p'(\nu)$ cannot be expressed in terms of known functions, the direct technique (cf. Sect. VT.2.1)) cannot be applied. On the other hand, this function is defined on the interval $[0, \infty)$, hence, the rejection technique also cannot be used.

For our purposes it will be useful to change the variable ν to $y = \beta h \nu$ and consider the function $p(y) = y^2/(e^y - 1)$. As we are interested in the distribution function normalized to unity, we omit the coefficient $(\beta h)^{-2}$. Notice that the definite integral $\int_{20}^{\infty} p(y)dy$ is very small, hence we may consider $p(y)$ on the interval [0, 20).

To apply the rejection technique to $p(y)$ one should divide the interval [0, 20) into several subintervals selecting for each of them a positive number C (cf. Sect. VI.2.2). Unfortunately such modified rejection technique yields rather complicated code, and is still slower than the direct recalculation of random numbers.

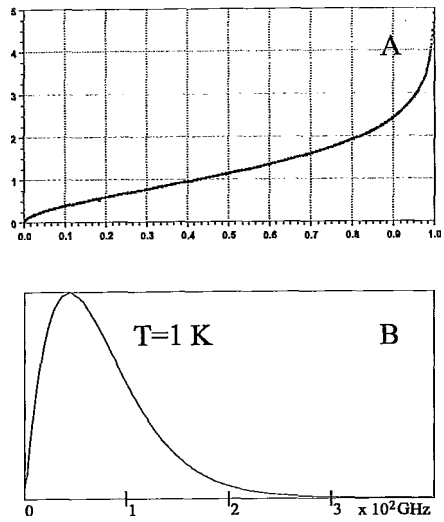

Fig. 2. The upper panel: the recalculation function $f_{pl}(u)$ corresponding to the Planckian distribution function of energies of radiated phonons. The lower panel: distribution of energies of phonons obtained with the help of f_{pl}. Over ten millions of phonons were generated

In our program, we decide to use the direct recalculation, with the recalculation function $f_{pl}(u)$ approximated by a table of numbers. Our recalculation function $f_{pl}(u)$ is depicted in Fig. 2.

The energy distribution function obtained with the help of $f_{pl}(u)$ is also shown in Fig. 2. We check that within numerical accuracy the plot of obtained distribution function is identical with the plot of function (74).

VII. PROGRAM DESCRIPTION

VII. 1. The architecture of the program

The program is written in C++ using OOP methods using the standard libraries. So it can be compiled and ran on any platform in the batch mode.

The program consists of two main objects - parser and experiment (Fig. 3). The parser object processes the input data and creates the queue of simulation scripts. The experiment encapsulates all the necessary elements of a simulated experiment (cf. Sect. Ill) as well as the simulation loop in which the phonons are sequentially processed.

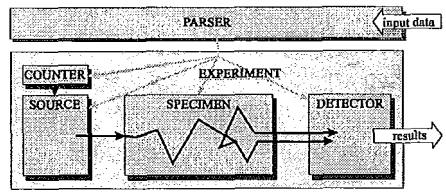

Fig. 3. The architecture of the program *MCAnScat*

The main loop of the program creates a phonon in the source, propagates it through the specimen and detects it at the boundaries of the sample.

The initialization of source, specimen and detector sub-objects is processed during creation of the experiment object. The constructor of the experiment forwards a set of the initialization data to the constructors of sub-objects. Errors detected during construction produce messages on standard output and set error flags which are tested at the beginning of the main loop.

An experiment can be assembled using different sources, specimens and detectors, depending on input data. Classes of the sub-objects are ordered using the inheritance relation. For creating a source, specimen or a detector as static objects with dynamically chosen type (class) we use handle-objects. A handle-object contains:

- a pointer to the object of base type of all allowed classes,
- the interface used in the main loop of the experiment,
- the constructor which creates the pointed object as the object of a proper class depending on some keywords in the initialization data.

The specimen propagates a phonon in a crystalline medium and contains the method of recalculating the phonon internal characteristics. The object specimen contains its own

propagation loop which propagates the phonon beginning with the injection of it by the source up to reaching the boundary by it.

Inside this loop a phonon is propagated step by step. Each step is terminated by an elastic collision, a down-conversion process, or when the phonon reaches boundaries. During each propagation step the phonon moves ballistically.

The time elapsing between successive collisions as well as the type of terminating event of a step is chosen randomly. When the type of event is determined, the characteristics of a finite phonon (or phonons) are chosen at random with the suitable probability densities (cf. Sect. V).

Now we shall describe the most important classes and the inheritance structure of objects. We shall not describe here the handle-classes as they have self-explaining structures.

VII.2. The program requirements

The program *MCAnScat* does not need any special computer and operating system capabilities. Even PC-AT 286 suffices to compile and run it, but then one can declare only output data arrays the size of which does not exceed 100 x 100. Since all internal calculations are performed using the double precision float numbers, a co-processor is recommended. The co-processor option should be set during the compilation. Processors i486 and PENTIUM contain the mathematical co-processor "on board". For PENTIUM based computers the cache memory speeds up simulations, provided the size of the output array does not exceed the cache size (each point on the detector array contains 4 bytes) and that no other processes are pending.

While the program is executed, it needs the memory for itself (its size depends on the compiler and compilation options), the output array (the declared size multiplied by the size of float data type) as well as approximately 50 KB for stack frame and temporary data structures. The amount of necessary memory depends also on the average number of phonon generations produced by down-conversion processes.

For UNIX workstations there are no specific requirements. Of course a large cache memory can speed up simulations. On DEC OSF (DEC3000,48MB RAM, 512KB CACHE, 2 GB HD, 200MB SWAP) we have found that simulations performed sequentially are much faster than many (more than eight) processes simultaneously. The program uses the floating point arithmetic, so it prefers processors optimized in this respect, for example the Alpha processor.

The program does not need graphic communication devices, and can be started using an alphanumeric terminal (e.g. using telnet).

VII. 2.1. Compilers

The program was compiled and tested on the PC386/486/PENTIUM (DOS 6.22 and DOS4GW DOS extender) and on the DEC3000 (DEC OSF 2.0). Using the Borland C 3.1, Watcom C/C++32 9.5b and Watcom C/C++ 10.6 compilers, we created Intel based application, and CXX compiler for DEC3000 Alpha application. The program does not use the graphic user interface (GUI), so the libraries dependent on system are not needed.

We also tried to compile and use this program on Silicon Graphics IRIS workstation, but the available compiler does not support some of the features used in the code. The program can be modified by the user to the version which can be compiled, but it may lose the compact and elegant form.

The complete set of source files contains the makefile for DEC CXX compiler (*makefile, dec*) and for Watcom 9.5b (*makefile.wat*).

VII. 2.2. Interface

An included additional interface allows the user to define in the interactive way the input data of experiments. This interface is written in the Visual BASIC programing language for WINDOWS platform.

VIII. PROGRAM USAGE

Vlil. i. Input data format

The input data are introduced in the command line while the *MCAnScat* is invoked. Each parameter corresponds to the name of the file which contains the data definitions. If some of the data should be changed, the user can overwrite it in the command line using the variables definition syntax. Such definitions must start with "-" sign and must not contain empty spaces. The overwriting is valid for all data files in the command line. This feature is useful, when the user wishes to prepare several experiments with the common values of variables (e.g. the number of phonons, geometry etc.).

The input data are introduced in the form of a set of definitions of variables as an ASCII file. The definition has the form *variablename = value*, where value can be a number (e.g. cl 1 = 12.26); a vector (e.g. s*ourcepos* = 0.03, 0.02, 0.05), a position on the plane or sphere (e.g. *detpos* = 0.12, -0.3; a size (e.g. *array* = 20 x 20); a crystallographic direction (e.g. *xaxis* = <3, 1, 1>) and a type (e.g. *detector = energy).*

A variable definition must not contain any white characters (empty spaces, tabulators, new lines, etc.).

VIII. 1,1. Units of measurements

VIII. 1.1.1. Ballistic motion

The elastic constants are expressed in 10^{11} x dyn/cm^2, hence

$$C_{rs} = [C_{rs}] \times 10^{11} \times \frac{\text{dyn}}{\text{cm}^2} \tag{75}$$

where (here and later on) numerical dimensionless coefficients are indicated by the square brackets. The mass density ρ is expressed in g/cm^3

$$\rho = [\rho] \times \frac{\mathrm{g}}{\mathrm{cm}^3}. \tag{76}$$

All introduced velocities - the phase velocity, components of the group velocity and the Debye velocity are in given in cm/s and are proportional to the coefficient 10^5. According to Sect. IV. 1.1. for isotropic media

$$c_\sigma = [c_\sigma] \times 10^5 \times \frac{\mathrm{cm}}{\mathrm{s}}, \ (\sigma = l, t), \tag{77}$$

where

$$[c_t] = \sqrt{10\frac{[\lambda + 2\mu]}{[\rho]}} \qquad \text{and} \qquad [c_l] = \sqrt{10\frac{[\mu]}{[\rho]}}.$$

In agreement with Eq. 14 for cubic media we introduce the coefficient

$$[c] = \sqrt{10\frac{[C_1]}{3[\rho]}}.$$

This means that $[c(\hat{K})] = [c]\,\tilde{c}(\hat{K})$ and

$$[c_D] = [c]\left\{\sum_j \int_{4\pi} \frac{\mathrm{d}\hat{k}}{4\pi}\,\tilde{c}^{-3}(\hat{K})\right\}^3. \tag{78}$$

A phonon $\hat{K}$ travels across a distance $d = [d]$ cm during the time interval $[t_d]$ μs, where

$$t_d(\hat{K}) = \frac{10[d]}{[c]\tilde{v}(\hat{K})}. \tag{79}$$

VIII. 1.1.2. Elastic scattering

Consider the mean collision frequency τ^{-1} (ω) (35). It is proportional to the volume of the unit cell $v_0 = [v_0]$ x 10^{-24} cm^3, to the linear frequency $\nu = [\nu]$ x 10^2 GHz and to the Debye velocity $c_D = [c_D]$ x 10^5 cm/s. Since the coefficient $\tilde{g}$ (36) is dimensionless this means that

$$\tau^{-1}(\nu) = [\tau^{-1}(\nu)] \times \mu\mathrm{s}^{-1}, \tag{80}$$

where

$$[\tau^{-1}(\nu)] = 4\pi^3 \frac{[v_0]\tilde{g}[\nu]^4}{c_D^3} \tag{81}$$

VIII. 1.1.3. Down-conversion processes

Using Eqs. (61) and (64) we obtain

$$\tau_i^{-1} = [\tau_i^{-1}] \times \mu s^{-1}, \qquad (i = L \to L + T, \quad L \to T + T), \tag{82}$$

where

$$[\tau_{L \to L+T}] = 12.8 \frac{[v]^5}{[\rho]^3} \frac{(\delta^2 - 1)}{[c_l]^9} \left([2[\beta] + 4[\gamma] + [\lambda] + 3[\mu])^2 I_{L \to L+T}(\xi_0)\right), \tag{83}$$

and

$$[\tau_{L \to T+T}] = 10 \frac{1.055\,\pi^4 [v]^5}{[\rho]^3 [c_l]^6 [c_t]^3} [I_{L \to T+T}(\xi_1, \xi_2)]. \tag{84}$$

This means the $\tau(v)$, τ_i $(i = L \to L + T, L \to T + T)$ are measured in μs.

Table II. Chosen units of measurements

Quantity	Notation	Units
Atomic mass	A	$[A]$
Density	ρ	$[\rho]$ g/cm^3
Elastic constants	C_{ij}	$[C_{ij}] \times 10^{11}$ dyn /cm^2
Length	d	$[d]$ cm
Phase velocites	c	$[c] \times 10^5$ cm/s
Phonon energy	w	$[w] \times 10^2$ GHz
Temperature	T	$[T]$ K
Time	t	$[t]$ μs
Volume of elementary cell	v_0	$[v_0] \times 10^{-24}$ cm^3

Chosen units of measurements are collected in Table II.

VIII.2. Types of the samples

The user can define several types of samples. The value of variable *crystal* contains the shape of the sample and the type of medium symmetry separated by commas. For the shape one can declare *sphere, parallelepiped, cylinder* or *infinite* (a medium without boundaries). For the medium symmetry one can declare *isotropic* or *cubic.* The list of shapes and symmetries can be extended by the user.

VIII.2.1. Laboratory versus crystallographic coordinate systems

The three fourfold crystalline axes of a cubic medium define the coordinate system. Orientation of *x (xaxis)* and z (*zaxis*) axes of laboratory coordinate system with respect to

the medium are characterized by the Miller indices. The Miller indices of the remaining axis are calculated automatically. In the case of a perpendicular parallelepiped or a cylindric sample the related sample planes are perpendicular to the laboratory coordinate system axes (axis). The orientation of an isotropic medium is arbitrary.

VIII.2.2. The source

- Spectral composition of radiated phonons:
  (1) Monochromatic (*source = monochromatic).* The user defines the energy $w = hv$ (variable *w*).
  (2) Planckian *(source = planckian).* One should set the temperature *T (temp).*
  (3) For all types of sources the user can define the amount of phonons of different polarizations using the variables *l*, *tf*, *ts.* The probability of choosing a phonon of the given polarization *j* is *j/*(1 + *tf*+ *ts),* where *j* - *l, tf, ts.*
- Geometry of the source:
  Several types of source geometries are allowed, namely
  (1) Point-like, located at the point $\mathbf{r}_v$ *(src)* inside the specimen, while the wave vectors of radiated phonons belong to the body angle 4π.
  (2) Rectangular, located on the bottom plane (this can be used for parallelepiped and cylinder samples only), with the center at $\mathbf{r}_b$ *(src)* and the size *(ssize).* Phonon wave vectors belong to 2π.
  (3) Point-like, wave vectors that belong to a cone $d\Omega_s$ *(sangle)* directed along axis $\hat{\mathbf{s}}$ *(sdir)* in the reciprocal space.
  (4) The extended source is treated as a continuous set of partial point sources. The probability of the generation of a phonon at the given point is assumed to be uniform.

The program checks the introduced data and determines the type of source.

VIII. 2.3. The size of the sample

- For parallelepiped one defines sizes along *x, y, z* axes of laboratory coordinate system. The size can be defined by setting:
  (1) minimum and maximum coordinates values *(xmin, xmax; ymin, ymax; zmin, zmax),*
  (2) sizes *(xsize, ysize, zsize)* - the origin of Cartesian coordinate system is located in the center of parallelepiped,
  (3) sizes and minimum (or maximum) values.

One can combine the above methods.

- For sphere one defines the radius (*r*) and the center coordinates *(center).*
- For cylinder one defines the height in the same way as z size of the parallelepiped, the radius *r* and the *x, y* coordinates (*rxy*) of the cylinder axis.
- For an infinite medium there are no size variables to be defined.

VIII.2.4. The set of medium characteristics

- For reasons described previously [8] we restrict ourselves here to the case of cubic crystals and isotropic media. So according to Sect. IV. 1.1 the set of the second order elastic constants consists of C_{11}, C_{12}, C_{44} or C_{11}, C_{12} respectively (the variables *c*11, *c*12, *c*44). The crystalline density is ρ *(rho)*.
- If one wishes to include phonon down-conversion processes, one should define the third order elastic constants. They can be defined in two ways:
  (1) by the set of two — α, γ of three parameters - α, β, γ (variables *ra, rb, rg)* (cf. Sect. V.4);
  (2) by the set of third order elastic constants C_{111}, C_{112}, C_{123}, C_{144}, C_{166}, C_{456} (variables *c*111, *c*112, *c*123, *c*144, *c*166, *c*456) (cf. [37,25])
  Internally the program uses parameters *rb, rg.*
- If one wishes to include phonon scattering by point mass defects one should define:
  (1) Volume of the unit cell v_0 (variable *v*0).
  (2) For lattices with basis:
    (a) Number *s* of atoms in the unit cell (variable *s*). These atoms are enumerated by the index $\sigma(\sigma = 1, \ldots, s)$ (cf. Sect. V.1)
    (b) Number *i* of atoms substituting the σ-th atom of the unit cell and their atomic numbers A^i_σ as well as their abundances f^i_σ *(isigma, aisigma,flsigma).*
  (3) For Bravais lattices containing substitutional (isotope) atoms of one kind:
    (a) the mass of host M_h and of substitutional (isotope) atom M_i - *{mh, mi),*
    (b) the concentration *c* of substitutional atoms (variable *c).*

In place of above data, one can use g_{imp} (*impurity*).

VIII. 2.5. Detection devices

Our detectors integrate signals. Detectors giving phonon patterns integrate over time. Detectors giving time-of-flight spectrograms integrate signals over the area of the detector surface.

- Resolution — For all kinds of detectors, one defines the resolution as the number of points comprising a pattern (e.g. *patternsize* = 256 x 256 for phonon patterns or *patternsize* = 1000 for time-of-flight spectrograms).

- Sensitivity - Due to the phonon focussing effect (cf. [8]) the strength of signals can differ by orders of magnitude. Generally, the interval of integrated signal amplitudes *I* ranges from the lowest $I_{\min}$ to the largest $I_{\max}$ detected values. To reveal the weak signal structures one should define the range (I^d_{dmin}, I^d_{dmax}) of the signals to store them as the output data. All values outside of this range will be stored as $I^d_{\min}$ (if $I < I^d_{min}$) or as I^d_{max} (if $I > I^d_{max}$). This can be achieved by defining:
  (1) The variable *overdrive* (*Idmax = overdrive Imax.* If *Idmin* is negative *Idmin = overdrive Imin,* otherwise *Idmin* = 0).

(2) Variables *absolutemin, absolutemax* (they define the minimal and maximal detected signal directly).

(3) Variables *relativemin, relativemax* (they define the ratio *Idmin = relativemin Imin; Idmax = relativemax Imax*).

VIII. 2.5.1. Types of detectors for limited specimen

There arc two different kinds of phonon beams spectroscopics - the time-of-flight and phonon images spectroscopy. So generally, for limited specimens the user has two types of detectors at their disposal giving respectively

- time spectrograms (*detector = time*)
- energy *(detector = energy*) and quasi-momentum (*detector = quasimomentum*) focussing patterns.

Similarly as for the source, the user should define the position and the size of the square detector (the center of the detector - *dpos;* the side length - *dsize*). Namely:

(1) For parallelepiped these data are in suitable units of length and the detector is placed at the top side of the parallelepiped.

(2) For the sphere of radius r (in cm) one uses spherical coordinates θ, ϕ (both in radians).

(3) For cylinder of radius r (cm) one uses cylindrical coordinates ϕ (in radians), z (in cm).

If those values are not defined, the detector covers the whole:

(1) top side of a parallelepiped,

(2) surface of a sphere,

(3) surface of revolution of a cylinder.

When *detector = time* the user defines the time gate $[0, t_g]$ (*tgate*), *tgate* is in μs.

When *detector = quasimomentum* the user defines the, direction $\vec{\eta}$ of components of quasi-momenta.

VIII. 2.5.2. Detectors for infinite media

To simulate the motion of phonons in an infinite medium we have prepared the special detector (*detector = tracer*) which allows for following, during the selected finite time interval ([0, *tgate*]), the track left by each radiated phonon. Two ready-to-use detectors produce the number (*trace = number*) and the energy (*trace = energy*) of phonons integrated over a selected body angle (the variables *dangle* and *ddir*) as a function of time.

VIII. 2.5.3. The count of phonons

The number of generated phonons in simulation experiments is defined by the user (the variable *count).*

VIII. 2.5.4. The output file

Setting the variable *fileformat* the user specifies the type of the output file. Its name may be defined using the variable *outfile.* If the output file name is not defined, the names of the output

and input file have merely different extensions. The default extension depends on the output file format, namely

*.ps - for file is in Adobe 1.0 PostScript format (*fileformat = postscript*),

*.byt - for the array of one-byte values [0,255] (*fileformat = byte_array*),

*.txt - for the ASCII text format (*fileformat = ascii*).

The header in (*fileformat = byte_array*) and (*fileformat = float_array*) contains the size of the pattern (or number of points in line) written as an ASCII text.

VIII. 2.5.5. Output data file format

The user can select one of four output data file formats: PostScript, byte array, float array, and text.

The PostScript output file format is the proper PostScript Adobe 1.0 format, and contains the bitmap representing the detector response (energy and quasi-momentum detectors) or the signal plot (detector for time-of-flight spectroscopy).

The byte and float arrays include a 16-byte header, which contains the data size (i.e. the size of the array representing data) written as ASCIIZ text (e.g. "256 x 256"). If an output file includes the plot data, the last byte in the header contains "*l*" (line). The data succeeding the header are sequentially stored as chunks of bytes (byte pattern) or 3 + 1 float values (float pattern) with no end-of-line separators. The values are normalized to the range [0,255] for byte array and [0, 1) for floats.

An ASCII output file contains the header with the size description (first line of the text), and the detector response values - on separate lines. There are no special separators for the end lines of the data.

One can import the PostScript files directly into text editors and (or) graphic presentation packages. The binary file formats are designed for future use of the data in applications written by the user. The text file format can be used by any spreadsheet as import data.

VIII.3. Test runs

VIII. 3.1. Propagation of ballistic pulses in GaAs

In computer experiments on ballistic propagation of phonons in GaAs described here (cf. Fig. 4), phonons are sequentially generated by the source placed on the (001) crystalline plane of a GaAs specimen (for which we have chosen the thickness $d = 0.2$ cm which is characteristic for GaAs substrates used in MBE technology). We also assumed that the source is placed in the center of the Cartesian coordinate system. Its z-axis is perpendicular to (001) plane in which lie the x- and y-axes. We chosen the typical frequency of phonons $\nu = 1.5$ THz. A small detector of phonons is placed on the opposite side of the platelet. In our computer experiments it has the form of the square of size $l = 0.2$ cm, therefore it subtends angles $\Delta\phi_{det} \lesssim 5.7^{\circ}$. The data used in our computer experiments are collected in Table III.

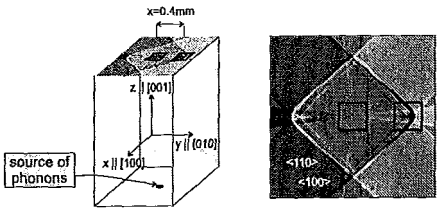

Fig. 4. Schematic illustration of the experiment on phonon beams, and (b) the map of the quasi-momentum density on the (001) lattice plane of GaAs obtained in computer experiments. White lines denote positive and black - negative, whereas the gray regions corresponds to the vanishing x-component of quasimomentum density. Phonon anemometers are represented by shaded squares. One of them is placed in the center of ST-box structure (*STB)* opposite to the source and the other one covers one of corners of *STB*

Table III. Data used in our computer experiments

The mass density [g/cm^3] and parameters of elasticity for GaAs [10^{11} dyn/cm^2]							
ρ	C_{11}	C_{12}	C_{44}	β	γ	λ	μ
5.32	11.26	5.71	6.0	-7.60	-6.73	4.30	4.86

The point like-pulsed source generating monochromatic phonons is located in the centre of the of the base and it radiates wave packets of phonons with the frequency ν, which we have taken 1.5 THz, into the body angle 2π. We assume that the initial distribution of directions of phonon wave vectors is isotropic. For simplicity we assume also that the probabilities to radiate a phonon *LA, FTA* and *STA* do not differ. Fig. 5 depicts the typical response of a bolometer to a pulsed beam of phonons.

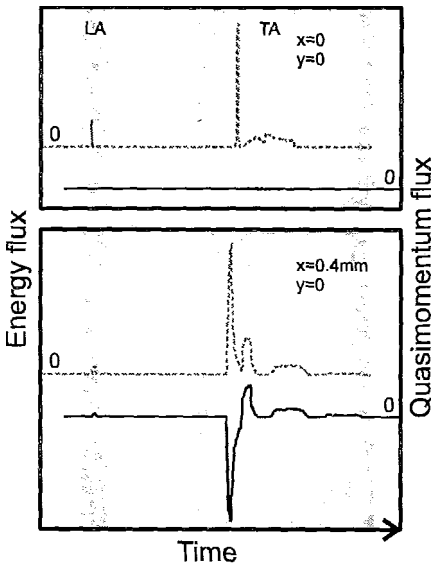

Fig. 5. Time-of-flight spectrograms for GaAs obtained in computer experiments. Detector placed (i) in *STB* center (upper panel), (ii) at *STB* corner (lower panel). Upper curves - energy, lower curves - quasi-momentum

In the ballistic regime of propagation of phonons we obtained the map of total energy density falling onto specimen surface. In agreement with results of real life [17] and computer

experiments [18] in Fig. 6 one sees the caustic lines with slow transverse box (*STB*) structure encircling the pattern center (cf. also Fig. 4). This energy density map serves us as the reference pattern used in the computer experiments on the quasi-momentum transport.

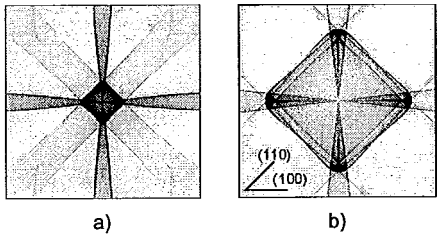

Fig. 6. (a) The map of the energy density obtained in computer experiments with a set of bolometers lying in (001) lattice plane of GaAs. (b) Caustic lines form the *"ST*-box" structure

In Fig. 7 we show the dependence of the arrival times of various phonon modes on the detector placement for the bolometer scanned along two selected directions. The arrival time of *LA* mode is a continuous and increasing function of time in agreement with geometrical conditions. Since for *LA* mode the slowness surface is almost spherical, experimental points for both directions lie on the same curve. *TA* modes behave quite differently. For both directions the arrival time of the leading front of corresponding pulses decreases with the growing distance from the center of the top surface of the parallelepiped (cf. Fig. 7). These findings are in excellent agreement with our real experiments and numerical calculations [40],

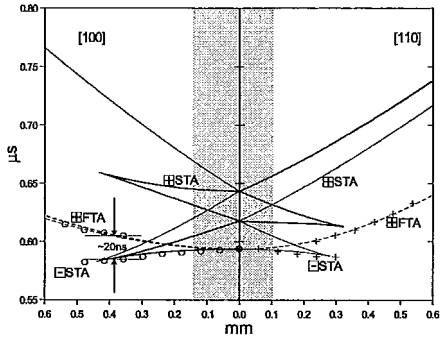

Fig. 7. Calculated dependence of *TA* modes arrival times on detector shift along [100] (left panel) and [110] axes (right panel). Solid lines - *STA,* dashed lines *FTA* modes. Thick lines indicate several modes moving with the same group velocities. Detector placed in the *STB* center registers all modes arriving at various time instants within the shaded stripe. Daggers and circles denote results of computer experiments. Signs ahead of the mode indices mark the sign of x component of quasi-momentum

VIII.3.2. Computer experiments on the diffusion of phonons in a sphere

Suppose that one deals with a solid with crystalline lattice having one atom in each unit cell and that the specimen has the form of the unit sphere. The source of phonons is located at the center of this sphere. Consider computer experiments on the phonon diffusion related to then-scattering by point mass defects. The parameter which distinguishes different experiments is α-factor defined by Eq. (35), which is proportional to the defects concentration c_{imp} (cf. Eq. (38)).

According to Eqs. (35), (51) the diffusion constant D is inversely proportional to $\tilde{g}$. In each computer experiment we used the same initial number of phonons N_v. The computer counts

the number of scattering events suffered by each injected phonon. In this way one obtains ng — the average number of collision events for a given $\tilde{g}$.

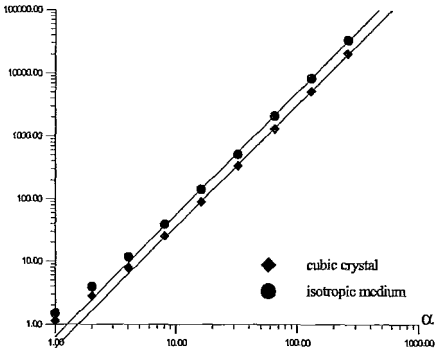

Fig. 8. The dependence of mean number of scattering events as a function of the parameter α (cf. Eq.(35)) for diffusive motion of phonons in the unit sphere

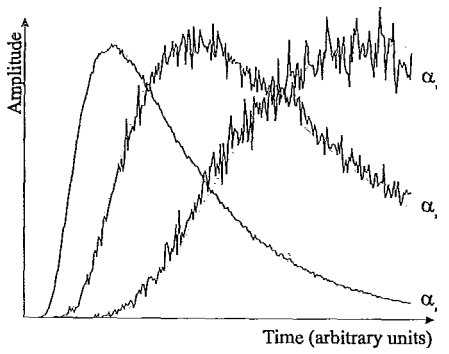

Fig. 9. Shapes of phonon pulses for different values of the parameter α (cf. Eq. (35)) for the diffusive motion of phonons in the unit sphere. Each maximum is normalized to its maximal value. The smooth lines correspond to theoretical curves (Eq. (55)). Erratic lines represent results of computer experiment for cubic elastic media $(\alpha_1<\alpha_2<\alpha_3)$

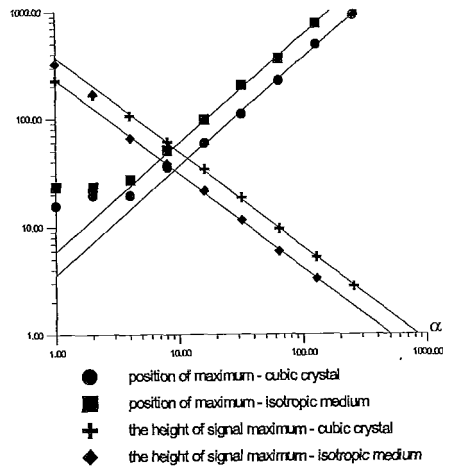

Fig. 10. The dependence of the position and height of the maxima of phonon pulses for the different values of the parameter α (cf. (35)) for diffusive motion of phonons in the unit sphere. For small values of α one deals with crossover between ballistic and diffusive motion

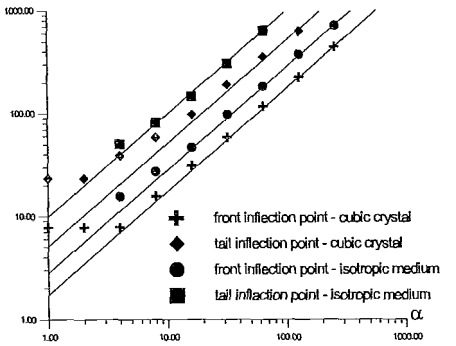

Fig. 11. The dependence of positions of the inflection points of the phonon pulses on the value of the parameter α (cf. Eq. (35)) for diffusive motion of phonons in the unit sphere. For small values of α one deals with crossover between ballistic and diffusive motion

Suppose that an erratically moving phonon passed the distance L during the time interval t_L. The mean free path $l \sim v\tau$. In the fully developed diffusive regime the mean number of collision

events $ng = t_L/\tau$ is proportional to $(L/l)^2 \sim \propto \tilde{g}^2$, hence $ng \sim g^2$. In Fig. 8 we show the dependence of ng on $\tilde{g}$ obtained in our computer experiments.

We considered the diffusion with the boundary condition given by Eq. (53).

In agreement with Sect. V.3. we assume that at the sphere boundary the value of number of phonons $N(r = R = 1, t)$ vanishes for any instant of time and only the flux density of phonons (Eq. (55) contains useful information. In Fig. (9) we show the flux $j(r = R = 1, t)$ normalized to its maximal value

$$j_{\max} = \sup_{T>0} j \ (r = R = 1, t)$$

as a function of time for different values of $\tilde{g}$. We see that for small values of $\tilde{g}$ curves have the form of narrow peaks and are smooth, while for large values of $\tilde{g}$ curves are broad and erratic. This effect can be easily explained. Simply, the same amount of phonons is concentrated on time intervals of different lengths and the normalization magnifies the fluctuations. We see that experimental and theoretical curves fit very well.

According to Sect. V.3. the arrival times of pulse maxima and positions of the inflection points are proportional to $\tilde{g}$, and then maxima are inversely proportional to $\tilde{g}$. Indeed, such dependencies are observed in computer experiments depicted in Figs. 10 and 11.

Thus, we conclude that when phonons of the beam suffer a large enough number of collision events, the propagation of beam becomes purely diffusive. In our experiments that happened approximately after 20 collisions ($ng \gtrsim 20$).

VIII.4. Inclusion of inelastic processes

Assume that besides the elastic scattering processes one allows also the phonon down conversion processes (cf. V.4). We performed suitable simulation for GaAs with about 10^6 phonons. In the absence of down-conversion processes one observes the typical diffusive pulse related to strong elastic scattering (Fig. 12, broken line). In result of the three phonon processes, on the front of the broad pulse one notices a strong maximum (Fig. 12, full line). It is related to low energy transverse phonons, which are weakly scattered by point mass defects. The tail of the diffusive pulse is also distorted. Danilchenko et al [34] performed similar experiments on isotropic elastic medium corresponding to GaAs.

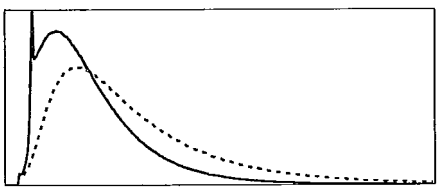

Fig. 12. Phonon down-conversion processes transform the diffusive pulse (dashed line). In the front of the pulse one sees a weak maximum related to longitudinal phonons and a strong one due to transverse phonons

Program summary

Title of program: *MCAnScat*

Program obtained from: CPC Program Library. Queen's University of Belfast, N. Ireland (see application form in this issue).

Licensing provisions: Person requesting the program must sign the standard CPC non profit use license (see license agreement printed in every issue).

Computers: IBM PC/AT 386 with numeric co-processor, IBM PC/AT486, PENTIUM, DEC 300 Alpha AXP.

Operating systems or monitors under which the program has been tested: Unix, Windows NT, DOS with DOS4GW extender

Programing language used: C++

Memory required to execute with typical data: 0.2 Mwords + 0.1 - 2 M words for data storage

No. of bits in a word: 32.

No. of processors used: 1

Has the code been vectorized: No.

Keywords: heat pulses, ballistic and diffusive transport of phonons, phonon down-conversion processes, cubic crystals, Monte Carlo computer experiments.

Nature of physical problem: Phonon beams are used for studies of various characteristics and properties of crystalline solids such as surfaces of constant energy or interaction of phonons with low dimensional gases of charge earners *(*1*D* and 2*D* gases of electrons and holes) [42], Their introduction greatly expanded the study of thermal transport in crystal by permitting the experimentalist to isolate particular phonon modes. Such studies provide a deeper understanding of properties of condensed matter. Simultaneously their results are of importance for development of modem technologies.

Usually ballistic phonons which propagate in crystalline media freely (without scattering) are considered. With such beams one investigates mainly the strong anisotropy of phonon currents being the result of phonon focussing. This interesting phenomenon can be studied by means of our program *MCFoc* [8].

However, phonons of beams can split and merge with thermal phonons and interact with quasi-particles of different kinds, defects and wells of specimens [7]. Using the massive dislocation-less, mono-crystalline, good-quality specimens of dielectrics and semiconductors at temperatures T much lower than the Debye temperature θ_D, one can eliminate most of scattering mechanisms. Nevertheless, even in lowest temperatures phonons can spontaneously decay and as a rule the specimens are not isotopically pure and contain other point mass defects (e.g. substitutional atoms) which scatter phonons (for review cf. [13]). So generally, propagating phonon beams contain both ballistic and scattered components. The quantitative comprehension of this latter component is important for the understanding of experimentally obtained

time-of-flight spectrograms and focussing patterns, which is particularly important for designing phonon based detectors of elementary particles [43].

For $T \ll \theta_D$ coalescence processes are very rare (cf. [7]), so the most probable process is the spontaneous down-conversion of phonons belonging to the beam to pah s of daughter phonons of lower energies. This means that beams propagating in media gradually change then spectral composition [44]. The time-of-flight spectrograms and phonon images allow for studying such changes [17]

Method of solution: Because no analytic solutions exist to the problem of transport of beams of decaying phonons which propagate in an anisotropic medium containing scattering centers, one has to resort to Monte Carlo calculations to obtain the insight. Hence, rather than solving problem using postulates and analytic methods we *model* the environment of the problem and simulate the evolution of the distribution function of phonons and their currents in a manner described by a set of random numbers.

Since for anisotropic media down-conversion processes are rather complex, we include them into our program in the simplest approximation. Namely, we assume that they occur in an equivalent isotropic medium [25,26], However, differently than in [34, 44] the propagation of phonons between successive phonon interaction acts is anisotropic. The elastic scattering events are anisotropic too.

In order to detect and remove possible errors in the Monte Carlo code we need special cases to check, in which theoretical estimates would be available. *The check calculations experiments were performed on ballistic gases of phonons and on systems in which down-conversion processes were prevented and elastic scattering is all that is permitted.* In contrast to Lax et al [1] we previously obtained some exact results for diffusive propagation of phonon beams in these media. We also *study the diffusive motion of down-converting phonons.*

Acknowledgments

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