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SURFACE INFLUENCE ON THE PHONON-PULSE PROPAGATION IN HEXAGONAL CRYSTALS

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The propagation of short phonon-pulses in crystals has become the standard method to study crystalline materials [1,2]. A theoretical description of this phenomenon was initiated by Kwok [3]. However, the influence of the surface of a sample has not been taken into account so far. This question is the subject of this note. We report our results for hexagonal crystals. This is the only case when the Christoffel equation has analytical solutions for any wave-vector direction $\vec{k}/|\vec{k}|$ [4]. This description via anisotropic continuum acoustics is fully justified at low temperatures, at which phonons propagate ballistically. Our description of the phonon-pulses propagation is based on the solution of the Boltzmann-Peierls [5] equation for the space- and time-dependent phonon distribution function $\delta f(\sigma,\vec{k};\vec{r},t)$ in the presence of an external phonon source.A scattering of phonons by bulk imperfections is considered within the τ-approximation.The sample is taken as a rod having a circular cross-section with a radius d. The rod axis (z) is chosen to be parallel to the sixth-order crystal symmetry axis(C axis).In heat-pulse experiments,phonons are usually generated in a crystal by an adjacent heater(characterized by a temperature T_H)located at the front face of the sample.We have found,following Rösch and Weis [6], that the distribution of the generated phonons takes the form of a product of the Bose-Einstein distribution

$$n(\sigma,\vec{k}) = \{\exp[\hbar\omega(\sigma,\vec{k})/k_B T] - 1\}^{-1},$$

and the transmission coefficient $\tilde{T}(\sigma,\vec{k})$(taken here approximately as a constant $\tilde{T}$ [7]).

The heater-sample area is usually small as compared to the sample cross-section. Moreover, the duration of the phonon-pulse generation is much smaller than the time for passing the length L of the sample by a phonon. Thus, one can treat the heater approximately as a point source and the rate of phonon production in the sample can be written down in the following form

$$\left(\frac{\partial \delta f}{\partial t}\right)_s = A\tilde{T}\delta(\vec{r})\,\delta(t)\,n(\sigma,\vec{k}), \qquad (1)$$

where A is a constant.

The solution of the Boltzmann-Peierls equation

$$\left[\frac{\partial}{\partial t} + \vec{v}(\sigma,\vec{k})\,\vec{\nabla} + \tau^{-1}(\sigma,\vec{k})\right]\delta f(\sigma,\vec{k};\vec{r},t) = \left(\frac{\partial \delta f}{\partial t}\right)_s \qquad (2)$$

has the form

$$\delta f(\sigma,\vec{k};x,y,z;t) = A\tilde{T} e^{-\frac{z}{v_z \tau}} \delta(\vec{r} - \vec{v}t)\, n(\sigma,\vec{k}). \qquad (3)$$

Because elastic properties of hexagonal crystals are invariant with respect to arbitrary rotations about C axis, it is worth to write down the obtained solution in the cylindrical coordinates (r, ϕ, z):

$$\delta f(\sigma,\vec{k};r,z;t) = \frac{A\tilde{T}}{2\pi r} e^{-\frac{z}{v_z \tau}} \delta(r - jz)\, \delta(z - v_z t)\, n(\sigma,\vec{k}), \qquad (4)$$

here j stands for v_r / v_z with v_r denoting the radial component of the group velocity vector $\vec{v}(\sigma,\vec{k})$.

The presence of the side surface of the sample is taken into account by introducing the so-called fictitious sources of phonons. We assume, following Fuchs [8,9], that a fraction p of phonons incident upon the surface is specularly reflected. Recently, Taborek and Goodstein [10], have shown that remaining phonons are completely transmitted to the liquid helium in which a sample is immersed. For that reason, we consider only specularly reflected phonons. The trajectory plane of the phonon $(\sigma,\vec{k})$ is specified by its group velocity vector $\vec{v}(\sigma,\vec{k})$. The first two fictitious sources are marked in Fig.1. Taking into account all directions of wave vectors one gets the loci of fictitious sources as circles of radii $2nd\,(n = 1,2,3,\ldots)$ centered on the real phonon source. The first circle corresponds to phonons reflected from the side surface, only once, the second one to those which suffer two successive reflections, etc. The power of the n-th fictitious source is p^n times as small as the real source power. Summing up the distribution functions for all sources one finally gets the complete solutions of the Boltzmann-Peierls equation in the form

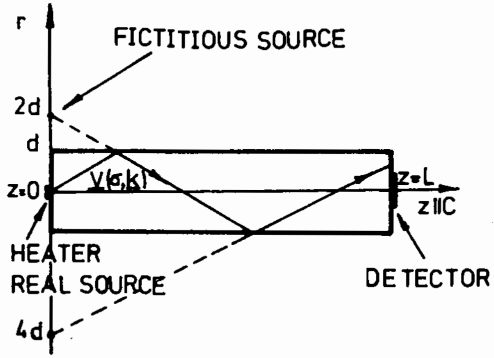
$$\delta f(\sigma,\vec{k};r,z;t) = \frac{A\tilde{T}}{2\pi r} e^{-\frac{z}{v_z \tau}} \delta(z - v_z t)\, n(\sigma,\vec{k}) \times$$
$$\times \{\theta(v_r) \sum_{n=0}^{\infty} p^n \delta(r + 2nd - jz) + \theta(-v_r) \sum_{n=1}^{\infty} p^n \delta(r - 2nd - jz), \qquad (5)$$

where $\theta(x)$ is the Heaviside function.

The energy flux of phonons of a polarization σ falling at a moment t upon the detector face (taken as a circle of a radius R) has the form

$$S(\sigma,t) = \int \frac{d\vec{k}}{(2\pi)^3} \int_0^R 2\pi r \hbar\omega(\sigma,\vec{k})\, v_z(\sigma,\vec{k})\, \delta f(\sigma,\vec{k};r,z=L,t), \qquad (6)$$

A scheme of a phonon-pulse propagation in a rod. The real phonon source is located at $r = 0$. The loci of the first two fictitious sources are marked at $r = 2d$ and $r = 4d$, respectively.



where $\omega(\sigma,\vec{k}) = kc(\sigma,\vec{k})$ is the frequency of the phonon $(\sigma,\vec{k})$. The simple form of the phase velocity $c(\sigma,\vec{k})$ for transverse mode $(\sigma = T)$ [4]

$$c(\sigma = T,\vec{k}) = [\lambda_{66} + (\lambda_{44} - \lambda_{66})(k_z/k)^2]^{1/2}$$

has allowed us to obtain $S(\sigma = T,t)$ in the analytical form

$$S(\sigma = T,t) = K(L)\frac{e^{-\frac{t}{\tau}}}{t^2}\{[\theta(t - \frac{L}{\sqrt{\lambda_{44}}}) - \theta(t - \sqrt{\frac{R^2}{\lambda_{66}} + \frac{L^2}{\lambda_{44}}})] +$$
$$+ \sum_{n=1}^{\infty} p^n [\theta(t - \sqrt{\frac{(2nd-R)^2}{\lambda_{66}} + \frac{L^2}{\lambda_{44}}}) - \theta(t - \sqrt{\frac{(2nd+R)^2}{\lambda_{66}} + \frac{L^2}{\lambda_{44}}})]\}. \qquad (7)$$

Here $K(L) = A\tilde{T}\pi^2 (k_B T_H)^4 L/(60\hbar^3 \lambda_{44}\lambda_{66})$ and $\lambda_{ij} = c_{ij}/\rho$ denote the reduced elastic constants.

Eq.(7) describes the shape of the energy flux falling upon the detector area as a function of time. In addition to the signal corresponding to phonons which have not been reflected from the sample surface, there exist also weaker signals, corresponding to phonons reflected n-time $(n = 1,2,3,\ldots)$.

The obtained results are very useful as the analytical guide for studying the irradiation of the detector face by phonons of the slow and fast modes. The strong phonons focusing occurring in the slow mode [11] has a dramatic effect upon the shape of the energy flux. For instance, for some hexagonal crystals and appropriately chosen length-to-radius sample ratios, the magnitude of the $n = 1$ peak may be much greater than the magnitude of the peak corresponding to the unreflected phonons. These and other results will be published in our forthcoming paper.

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Гнат А., Пашкевич Т., Петру З. E17-83-740
Влияние поверхностей на распространение импульсов тепла в гексагональных кристаллах

Изучается распространение фононных импульсов в области Кнудсена, т.е. с учетом рассеяния на поверхности образца. В приближении времени релаксации найдено решение уравнения Больцмана-Пайерлса. Получено аналитическое выражение для потока энергии поперечных фононов, падающих на поверхность болометра.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Hnat A., Paszkiewicz T., Petru Z. E17-83-740
Surface Influence on the Phonon-Pulse Propagation in Hexagonal Crystals

We study the phonon-pulse propagation in a rod of a hexagonal crystal in the boundary-scattering regime. The Boltzmann-Peierls equation is solved and the energy flux of transverse phonons falling upon a detector face is obtained in the analytical form.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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