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E17-85-674

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ANISOTROPY OF ISOTOPE-SCATTERING RATE IN CRYSTALS OF HEXAGONAL SYMMETRY

Submitted to the Second International Conference
on Phonon Physics, Budapest, 1985

1985

A number of experiments on the propagation of acoustic phonons have revealed anomalously long phonon life-times at low temperature[1]. Lax et al.[2] have shown theoretically that isotope-scattering rate of phonons in diatomic crystals (such as GaAs) which have one element isotopically pure depends strongly on the amplitude of vibrations of the impure element. They have suggested that the isotope scattering in multiatomic lattices may be weaker than that expected from usual theoretical treatments of monoatomic lattices, which can explain anomalously long-lived phonons (see also[3]).

The purpose of this paper is to show that also in monoatomic lattices (of noncubic symmetry) the isotope-scattering rate depends explicitly on the eigenvector of atomic displacement and thus it depends on the direction of phonon propagation. To present results in an analytic form, the crystal will be treated as an anisotropic elastic contimuum of hexagonal symmetry.

In a crystal in which isotopic atoms are distributed randomly on the lattice sites the scattering rate, or the reciprocal of the relaxation time of $(\vec{k}j)$-phonon scattered by isotopes, is given by[3]

$$\tau_j^{-1}(\vec{k}) = \frac{\pi g\, \omega_j^2(\vec{k})}{12\, N} \sum_{\vec{k}'j'} \delta\left(\omega_j(\vec{k}) - \omega_{j'}(\vec{k}')\right) \left| \vec{e}_j(\vec{k}) \cdot \vec{e}_{j'}(\vec{k}') \right|^2 . \quad (1)$$

Here $g = \sum_i f_i (1 - M_i/M)$, where f_i is a friction of unit cells with a mass M_i, and M is the averaged mass of unit cell. Polarization vectors are normalized in accord with $|\vec{e}_j(\vec{k})|^2 = 1$.

In the long wave limit the scattering rate can be written as a function of polarization vector with two constant parameters: the Debye velocity and the inverse cube of sound velocity weighted with the polarization vector,

$$c_D^{-3} = \frac{1}{3} \sum_j \langle c_j^{-3} \rangle \quad \text{and} \quad b^{-3} = \frac{1}{3} \sum_j \langle c_j^{-3} |e_j^z|^2 \rangle,$$

resp. In the case of pure transverse phonons, $j = T_1$, for which $e^z_{T_1} = 0$ the relaxation time is equal to

$$\tau^{-1}_{T_1}(\omega) = \omega^4 \cdot \frac{g \cdot v_0}{12\pi} \cdot \frac{3}{2+\Gamma} , \qquad (2)$$

where v_0 is a volume of unit cell. Scattering rates of quasilongitudinal ($j = L$) and quasitransverse ($j = T_2$) phonons are direction-dependent

$$\tau^{-1}_j(\omega\hat{k}) = \tau^{-1}_{T_1}(\omega) \cdot [1 + (\Gamma - 1)|e^z_j(\hat{k})|^2] , \qquad (3)$$

where $\hat{k} = \vec{k}/|\vec{k}|$.

Anisotropy parameter Γ defined by equality

$$\Gamma = 2 b^{-3}(c_D^{-3} - b^{-3})^{-1} , \qquad (4)$$

decides how strong the dependence on the polarization vector is. For the case of monoatomic cubic crystals or for isotropic medium $c_D^{-3} = 3b^{-3}$ and $\Gamma_{cub} = \Gamma_{isotr} = 1$. Square of the z-component of polarization vector appearing in Eq.(3) can be written as

$$|e^z_j(\hat{k})|^2 = \frac{1}{2}\{1 \pm W[W^2 + 4(C_{11}+C_{44})^2 \hat{k}_z^2(1-\hat{k}_z^2)]^{-\frac{1}{2}}\} , \qquad (5)$$

where

$$W = C_{11} - C_{44} - (C_{11} + C_{33} - 2C_{44})\hat{k}_z^2 .$$

Here C_{ij} are elastic constants. The plus sign corresponds to $j = L$ and minus to $j = T_2$.

When the angle Θ between direction of $\vec{k}$ and sixfold axis changes from 0° to 90°, the value of $|e^z_{T_2}|^2$ will increase monotonically from 0 to 1. Thus, the scattering rate of T_2 phonons increases monotonically for crystals with $\Gamma > 1$ and decreases for crystals with $\Gamma < 1$. In Table 1 monoatomic uniaxial crystals are classified with respect of their low temperature values of Γ.

T a b l e 1. Anisotropy parameter Γ of uniaxial crystals

	Cadmium	Hafnium	Helium-4	Hydrogen J = 1	Magnesium
Γ	2.1177	0.92036	0.64772	0.82180	1.13408
	Rhenium	Thallium	Titanium	Zinc	Zirconium
Γ	0.92412	0.38524	0.84891	2.2152	0.99796

Formula (3) suggests that the ratio τ_L/τ_{T_2} may change by factor 3 or 4 with changing the direction in such crystals as helium, cadmium, thallium and zinc.

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Received by Publishing Department
on September 17, 1985.

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Петру З. E17-85-674

Анизотропия рассеяния фотонов на изотропических примесях в гексагональных кристаллах

Исследована анизотропия рассеяния фононов изотопическими примесями в гексагональных кристаллах. Вычислена зависимость частоты столкновений длинноволновых фононов от направления волнового вектора. Введен параметр анизотропии Г, и показано, что частота столкновений квазипоперечных фононов растет /Г > 1/ или падает /Г < 1/ с ростом угла между направлением волнового вектора и оси симметрии. Квазипродолным фононам свойственно обратное поведение. Проведена классификация одноосных кристаллов по величине из низкотемпературного параметра анизотропии Г.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1985

Petru Z.K. E17-85-674

Anisotropy of Isotope-Scattering Rate in Crystals of Hexagonal Symmetry

Anisotropy of phonon scattering by isotope impurities is studied in crystals of hexagonal symmetry. The dependence of scattering rates of long-wave phonons on a wave-vector direction is calculated. The anisotropy parameter Г is introduced depending on which the scattering rate of quasitransverse phonons increases /Г > 1/ or decreases /Г < 1/ with increasing the angle between wave-vector direction and symmetry axis. The opposite behaviour takes place for the scattering rate of quasilongitudinal phonons. Monoatomic uniaxial crystals are classified with respect to their low-temperature values of Г.

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

Preprint of the Joint Institute for Nuclear Research. Dubna 1985