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Abstract

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ON THE ANISOTROPY OF THE MÖSSBAUER EFFECT

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It was noted earlier that the probability of resonant absorption (emission) of γ-quanta in noncubic crystals should possess a clearly pronounced anisotropy effect (see, for example, ([1])). Physically this is connected with the fact that the probability of phonon excitation depends on the direction of the recoil momentum of the nucleus relative to the crystallographic axes.

To estimate the magnitude of this effect, let us consider a simple lattice of the rhombic system, in which the atoms interact in a central and noncentral manner with their nearest neighbors (along the edges of the parallelepiped). For a certain relation between the parameters, such a lattice will pass into the simple lattices of the tetragonal and cubic systems.

From symmetry considerations it is easy to conclude that vibrations in the directions of the axes of the parallelepiped are independent. Therefore the secular equation splits into three independent equations of the form

$$m\omega_\alpha^2 = 2\sum_{\beta=1}^{3}\gamma_{\alpha\beta}(1-\cos\varphi_\beta), \qquad \alpha,\beta = 1,2,3, \tag{1}$$

where the diagonal elements of the matrix $\gamma_{\alpha\beta}$ are the central force constants, while the nondiagonal elements are the noncentral force constants corresponding to displacements along α for neighbors closest along the β axis.

The distribution function of the frequencies of the phonon spectrum for each branch can be determined by the same method as in the case of the simple cubic lattice (see ([2], [3])). In accordance with (1) we have:

$$g_\alpha(\omega^2) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\left\{-i\rho\omega^2 + i\frac{2}{m}\sum_{\beta=1}^{3}\gamma_{\alpha\beta}\rho\right\}\prod_{\beta=1}^{3} J_0\left(\frac{2\gamma_{\alpha\beta}}{m}\rho\right)d\rho. \tag{2}$$

The probability of the Mössbauer effect under resonant absorption of γ-quanta in a crystal is determined by the quantity $\exp\{-Z\}$, where

$$Z = R\frac{v_0}{(2\pi)^3}q^\xi q^\eta \sum_\alpha \int d^3f\, \frac{V_\alpha^\xi(\mathbf{f})V_\alpha^\eta(\mathbf{f})}{\hbar\omega_\alpha(\mathbf{f})}\,[2\bar{n}_\alpha(\mathbf{f})+1] \equiv q^\xi q^\eta T^{\xi\eta}. \tag{3}$$

(The notation is the same as in ([1], [3]); summation is carried out over repeated upper indices.)

The anisotropy of the effect is determined by the tensor $T^{\xi\eta}$, whose principal axes coincide with the crystallographic axes. If one takes into account that the polarization vector of the α-th branch $\mathbf{V}_\alpha$ is parallel to the α axis, then for the diagonal elements of the tensor we have

$$T^{\xi\xi} = \frac{2R}{\hbar}\int g_\xi(\omega^2)[2\bar{n}(\omega)+1]\,d\omega. \tag{4}$$

or, at an arbitrary temperature (the corresponding derivation for a cubic crystal is given in (3)),

$$T^{\xi\xi} = \frac{R}{2kT}\int_0^\infty \exp\left\{-\frac{\hbar^2}{2m(kT)^2}\left(\sum_{\alpha=1}^3 \gamma_{\xi\alpha}\right)t\right\}\theta(t)\prod_{\alpha=1}^3 I_0\left(\frac{\hbar^2\gamma_{\xi\alpha}}{2m(kT)^2}t\right)dt, \tag{5}$$

where $\theta(t)$ coincides with the Jacobi function of the third kind with argument $i\pi t$.

To estimate the anisotropy of the Mössbauer effect it is necessary to compare the values of $T^{\xi\xi}$ for different axes, taking into account the real parameters of the crystal.

Let us establish the relation between the elements of the matrix $\gamma_{\alpha\beta}$ and the elastic constants of the crystal. It can be shown that, within the framework of the model under consideration,

$$\begin{aligned}
\gamma_{11} &= \frac{c_{11}a_2a_3}{a_1}, & \gamma_{22} &= \frac{c_{22}a_1a_3}{a_2}, & \gamma_{33} &= \frac{c_{33}a_1a_2}{a_3},\\
\gamma_{12} &= \frac{c_{66}a_1a_3}{a_2}, & \gamma_{13} &= \frac{c_{55}a_1a_2}{a_3}, & \gamma_{23} &= \frac{c_{44}a_1a_2}{a_3},\\
\gamma_{21} &= \frac{c_{66}a_2a_3}{a_1}, & \gamma_{31} &= \frac{c_{55}a_2a_3}{a_1}, & \gamma_{32} &= \frac{c_{44}a_1a_3}{a_2}.
\end{aligned} \tag{6}$$

In the case of a tetragonal lattice (the c-axis coincides with axis 3), $a_1 = a_2$, $c_{11} = c_{22}$, $c_{44} = c_{55}$, and the number of independent elements of the matrix $\gamma_{\alpha\beta}$ is reduced to five.

Let us consider, for this lattice, the limiting case $T = 0$:

$$T^{33} = \frac{R}{k\theta} \sqrt[6]{\frac{81\pi}{2}}\, f \int_0^\infty \frac{1}{\sqrt{t}} \sin\left[(2+\xi_1)t + \frac{\pi}{4}\right] J_0(\xi_1 t) J_0^2(t)\, dt; \tag{7}$$

$$T^{11} = \frac{R}{k\theta} \sqrt[6]{\frac{81\pi}{2}}\, f \sqrt{\xi_4} \int_0^\infty \frac{1}{\sqrt{t}} \sin\left[(1+\xi_1+\xi_2)t + \frac{\pi}{4}\right] J_0(t) J_0(\xi_2 t) J_0(\xi_3 t)\, dt,$$

where

(8)

$$f = \left[\frac{1}{\sqrt{\xi_1}} + \frac{2}{\sqrt{\xi_2 \xi_3}}\, \xi_4^{3/2}\right]^{-1/3}, \tag{9}$$

$$\xi_1 = \frac{\gamma_{33}}{\gamma_{31}}, \qquad \xi_2 = \frac{\gamma_{11}}{\gamma_{13}}, \qquad \xi_3 = \frac{\gamma_{12}}{\gamma_{13}}, \qquad \xi_4 = \frac{\gamma_{31}}{\gamma_{13}};$$

θ is the Debye temperature for the tetragonal crystal under consideration, which is obtained from the low-temperature limit for the heat capacity,

$$\theta = \frac{\hbar}{k\sqrt{m}} \left[\frac{1}{18\pi^2}\left(\frac{1}{\gamma_{31}\sqrt{\gamma_{33}}} + \frac{2}{\sqrt{\gamma_{22}\gamma_{13}\gamma_{21}}}\right)\right]^{-1/3}. \tag{10}$$

To determine the effect in a real case and, most importantly, to estimate the anisotropy, the distribution of the crystal frequencies may be approximately approximated by functions obtained within the framework of the model under consideration using experimentally determined values of c_{ik}. Since function (2) possesses all the features of the general form characteristic of the frequency distribution of the phonon spectrum, and fixing the parameters (6) is in fact equivalent to specifying the moments of the distribution function, such an approximation for the analysis of the spectral integrals of interest to us apparently should be quite satisfactory.

Among monatomic noncubic crystals for which the Mössbauer effect is presently known, white tin is of greatest interest; it has tetragonal symmetry ($a \simeq 5.8$ Å, $c \simeq 3.15$ Å). For this crystal, the values of c_{ik} have recently been measured[4] for two temperatures: $T = 93^\circ$ K and $T = 288^\circ$ K (in fact the constants s_{ik} were measured; the transition to c_{ik} is carried out in the usual way). Using the values c_{ik} corresponding to $T = 93^\circ$ K, calculations of T^{11} and T^{33} were performed. The ratio of these quantities, which in fact characterizes the anisotropy, turned out to be $T^{11}/T^{33} \simeq 1.17$. Thus, the intensity of recoil-free emission along the c axis is greater than in the perpendicular direction. To determine the anisotropy directly of the magnitude of the Mössbauer effect, let us estimate the absolute value $T^{\xi\xi}$ (7) and (8); for this we shall use the value $\theta \sim 200^\circ$ K and the recoil-energy value $R = E_\gamma^2/2mc^2$ ($E_\gamma = 23.8$ keV). As a result, for the probability ratio at $T = 0$ (the source is assumed fixed) we find $w_3/w_1 \simeq 1.04$. If (5) is used, then the ratio w_3/w_1 can be analyzed for arbitrary temperatures. Direct calculations have shown that with increasing temperature the anisotropy effect changes little.

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References

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Note: Figure translations are in progress. See original paper for figures.