PHONON GAP IN ANISOTROPIC FILM AND EFECTS ON INTERNAL ENERGY AND SPECIFIC HEAT

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In reference |1| we analysed the phonon spectra of anisotropic film $a_x \approx a_y = a$; $a_z >> a$. *The translational symmetry is preserved in XY planes, while along the z-axis presence of the boundaries is taken into account.*

Dispersion law phonons in the above described structure is

$$E_{fl}(k) = 2\varepsilon\left(\sin^2 \frac{ak_x}{2} + \sin^2 \frac{ak_y}{2} + \cos^2 \frac{b_\nu}{2}\right)^{1/2} \qquad (1)$$

$$\varepsilon = \hbar\sqrt{\frac{C}{M}}\ ; \quad C = \frac{1}{3}\sum_\alpha C_{\alpha\alpha}\ , \quad \alpha = x,y,z\ ;$$

where $C_{\alpha\alpha}$ *- elasticity constant, M - mass of molecule,* $a_x = a_y = a$; $a_z >> a$ *- lattice constants.*

The values of b_ν *are determined by the transcendental equation:*

$$\cot\,(N_z+2)b_\nu = \frac{(1+\cos b_\nu)^2 + \frac{1}{2}}{(2+\cos b_\nu)\,\sin b_\nu}\ ; \qquad (2)$$

$0 < b_\nu < \Pi$; $\nu = 0,1,2,\ldots,N_z$; $b_\nu \neq 0$;

N_z+1 *- is the number of layers of the film.*

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From (1) it is evident that due to boundary presence the phonon spectra have a gap. Practically it is impossible to verify this gap by measuring the dispersion law since instruments do not allow the type of measurements in the domain of extremely small k. In order to verify the presence of a gap it is wise to determine the specific heat of the system at low temperatures, and if the gap exits the specific heat of the film would drastically differs from the specific heat of the ideal structure of the same specimen (Boyd Veal-private communication).

At low temperature the low - energy phonos are relevant, and we take: $k_x = k_y \approx 0$ *and* $b_\nu \approx \Pi$.
Approximate solutions of the transcendental equation (2) are

$$b_\nu = \frac{\Pi}{N_z+2}\left(\nu + \frac{3}{2}\right); \quad \nu = 0, 1, 2, \ldots, N_z. \tag{3}$$

In accordance to the previously said we can take:

$$\cos\frac{b_\nu}{2} \approx \cos\frac{b_{N_z}}{2} = \cos\frac{\Pi}{2}\,\frac{N_z+3/2}{N_z+2} =$$

$$\cos\frac{\Pi}{2}\left(1-\frac{1}{2}\,\frac{1}{N_z+2}\right) = \sin\frac{\Pi}{4}\,\frac{1}{N_z+2} \approx \frac{\Pi}{4(N_z+2)} \tag{4}$$

such that (1) becomes

$$E_{fl} = (\varepsilon^2 a^2 k^2 + \Delta^2)^{1/2}, \tag{5}$$

where $\Delta = \frac{\Pi\varepsilon}{2(N_z+2)}$ *is the gap whies, as evident, decreases with the film thickness.*

Internal energy is given by the expression:

$$U_{fl} = 3 \sum_{k_x k_y} \sum_{\nu=0}^{N_z} \frac{E_{fl}(k)}{e^{\frac{E_{fl}(k)}{\Theta}} - 1} \tag{6}$$

After substitution of (5) into (6) and going over from sumation to integral we get U_{fl}, and the specific heat C_{fl} as temperature derivative:

$$C_{fl} = \frac{\partial U_{fl}}{\partial T} = \frac{3k_B}{2\Pi} N_x N_y (N_z+1) \Big[(\frac{\Delta}{\varepsilon})^3 \frac{1}{\tau} (e^{\frac{\Delta}{\varepsilon\tau}} - 1)^{-1} +$$

$$+ 3(\frac{\Delta}{\varepsilon})^2 \sum_{n=1}^{\infty} \frac{1}{n} e^{-n\frac{\Delta}{\varepsilon\tau}} + 6 \frac{\Delta}{\varepsilon}\tau \sum_{n=1}^{\infty} \frac{1}{n^2} e^{-n\frac{\Delta}{\varepsilon\tau}} + \qquad (7)$$

$$+ 6\tau^2 \sum_{n=1}^{\infty} \frac{1}{n^3} e^{-n\frac{\Delta}{\varepsilon\tau}} \Big] \; ; \; \tau = \frac{k_B T}{\varepsilon} << 1 .$$

It is necessary to compare (7) to the specific heat of the ideal structure. Dispersion law for phonons in ideal structure is

$$E_{id} = 2\varepsilon (\sin^2 \frac{ak_x}{2} + \sin^2 \frac{ak_y}{2} + \sin^2 \frac{ak_z}{2})^{1/2} . \qquad (8)$$

For the low energy phonons $k_x, k_y, k_z \approx 0$ and (8) becomes

$$E_{id} = \varepsilon ak; \; k = (k_x^2 + k_y^2 + k_z^2)^{1/2} . \qquad (9)$$

such that:

$$U_{id} = \frac{9N_{id}}{\Pi^2 \varepsilon^2} \zeta(4) k_B^4 T^4 ; \; N_{id} = N_x N_y N_z \qquad (10)$$

where: $\zeta(4) = \sum_{n=1}^{\infty} \frac{1}{n^4}$ is the Riemann's zeta function.

From (10) it follows:

$$C_{id} = \frac{36}{\Pi^2} \zeta(4) \; N_{id} k_B \tau^3 \qquad (11)$$

Comparing expressions (7) and (11) it is evident that analytical dependance of specific heat on non-dimensional temperature τ drastically differs - for film and bulk structure. These differences can be experimentally observed.

If we treat superconducting ceramic film as anisotropic film, it is understandable that the presence of the phonon gap can be one of the causes for higher T_c.

References:

[1] B.S.Tošić , J.P.Šetrajčić, R.P.Djajić, D.Lj.Mirjanić: Phys.Rev. B 36, 9094(1987; Int.J.Mod.Phys. B1,1001(1987): Int.J.Mod.Phys. B1,919(1988).