

Phonon interactions in quantum films

M. Arakelyan

Yerevan State University





Introduction



- ▶ Phonon technologies in nano and heterostructures are especially important for modern instrumentation. The question of the formation of bound states of excitations in such structures attracts much attention.
- ▶ The study of phonon interactions in models describing the properties of nanostructures will make it possible to control the scattering frequency, dissipation rate, resonance conditions, phonon mean free path, and control the evolution of a qubit in quantum computers and heterostructures. [1]. The phonon lifetime depends on temperature: with increasing temperature, the phonon lifetime decreases and for optical phonons in GaAs it ranges from several picoseconds (300K) to ten picoseconds (77K) [2]. Fig. 1, 2.

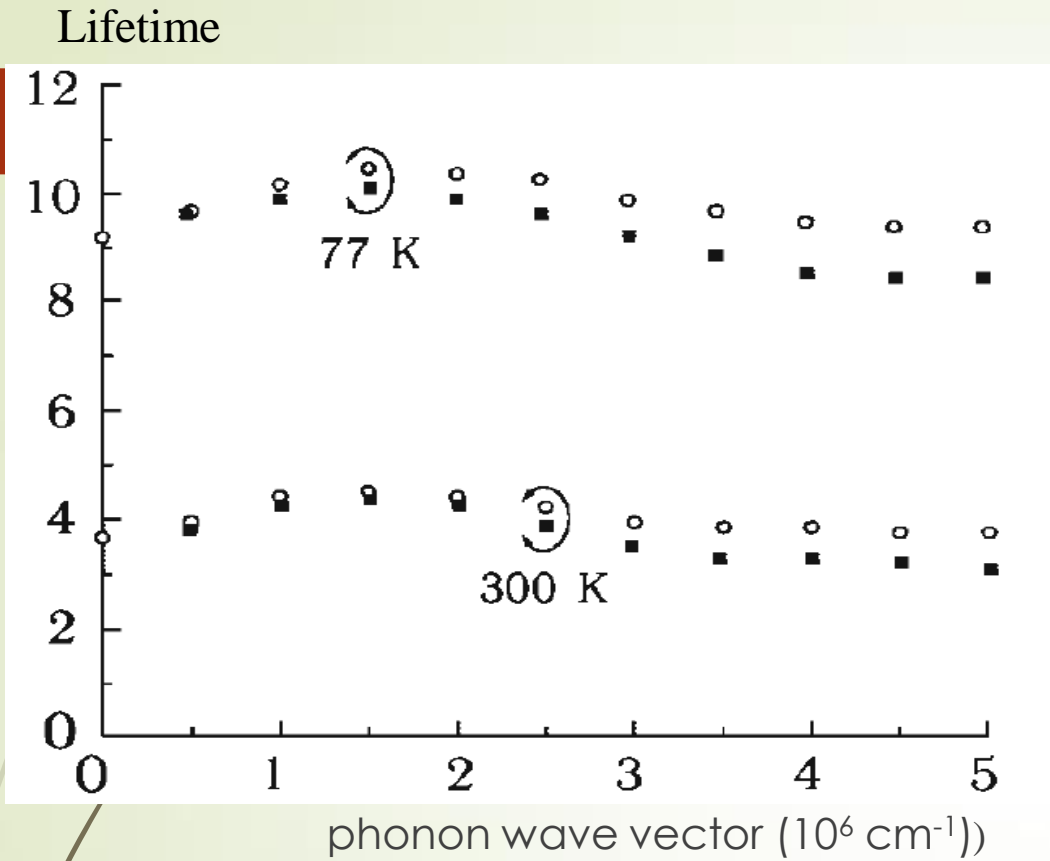


Fig. 1. Dependence of the lifetime of longitudinal optical phonons on the magnitude of the wave vector along the direction 100 (squares) and 111 (circles)

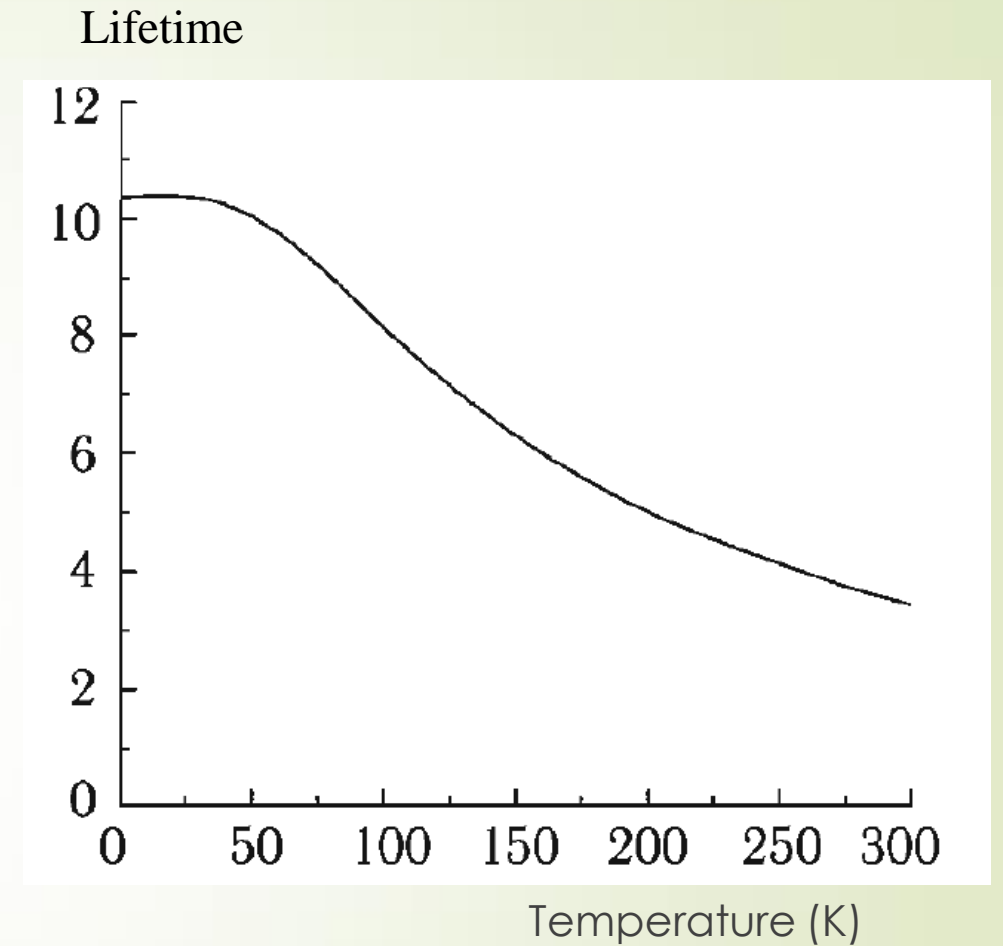
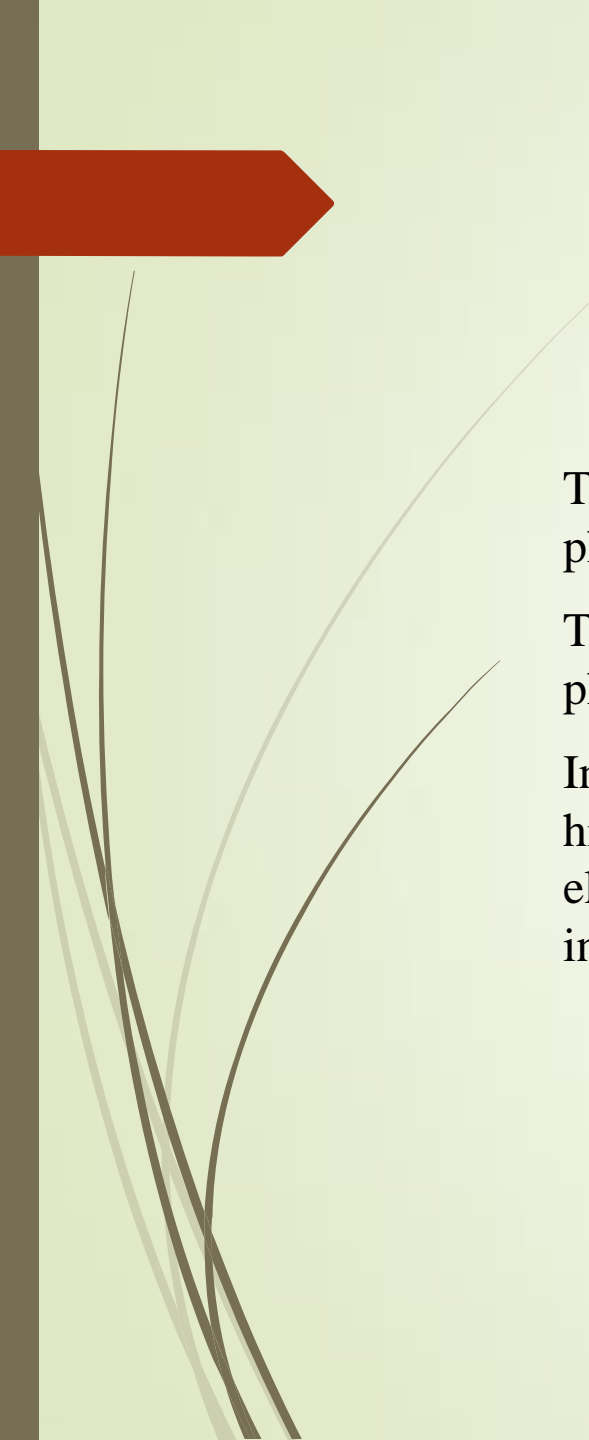


Fig. 2. Temperature dependence of the lifetime of a longitudinal optical phonon



Thus, in wide ranges of temperatures and wave vectors, the times of longitudinal optical phonons vary over a wide range

The carrier energy relaxation rate is strongly dependent on the lifetime of longitudinal optical phonons.

In addition, the phonon density in semiconductors under size quantization conditions is much higher than the phonon density in bulk samples. [2]. In turn, an increase in the energy of electron-phonon interaction leads to a decrease in the transition time between quantum levels in size-quantized systems [3], which increases the speed of working systems in devices.

Bound states of optical phonons

- Let us make the following assumptions: optical phonons do not have dispersion; crystal temperature is low

$$T \ll \varepsilon_{\Phi}$$

(ε_{Φ} is the energy of the optical phonon)

Under the following boundary conditions and the condition of unitarity of the matrix elements ζ of the transformation matrix from variables to the generalized coordinates characteristic of the film we can write (see, for example, [4])

$$\zeta_0 = \zeta_{(N_3+1)a} = 0, \quad \frac{2}{(N_3+1)} \sum \sin(qn) \sin(q' n) = \delta_{q,q'}$$

Bound states of optical phonons

- We obtain the dispersion Ω equation for optical phonons in the film:

$$\Omega = 2 \sqrt{\frac{\gamma}{\mu}} \left[1 - \frac{2\mu}{m_1 + m_2} \sin^2 \frac{q_3 a}{2} (1 + \cos^2 \frac{q_3 a}{2}) \right]; \mu = \frac{m_1 m_2}{m_1 + m_2};$$

where γ is the coefficient characterizing the forces of phonon interaction ($\gamma \ll 1$); the displacements 0 and $a/2$ of the atoms from the equilibrium positions and in the unit cell with the number n are indicated respectively. $\zeta_{n,1}, \zeta_{n,2}$, q_3 - the wave vector of the phonon in the direction of y , m_1, m_2 - the masses of the atoms of the unit cell. N_3 - the number of molecular layers in the y direction.

Bound states of optical phonons

- Next, the equation for the bound states of phonons in the film is obtained:

$$V(q) = \frac{2}{N} \sum_{m,n} \exp[iq_{\perp}(m_{\perp} - n_{\perp}) \sin(q_3 ma) / \sin(q_3 na)] V_{mn},$$

$$n_{\perp} = a_1 n_1 + a_2 n_2$$

where $V(q)$ - matrix element of the energy of interaction of particles «m» and «n» in the q representation.

- If we take into account the matrix elements of excitation transfer only between neighboring particles, then

$$V_{m,m+1} = V_{m-1,m} = V, \quad V(q) = 4V \cos(q_3 a) \cos(q_{\perp} a).$$

- After the transition from summation over to integration, the binding energy ε of phonons was found:

$$\varepsilon = \pm 4 \sqrt{\frac{A^2}{(N_3 + 1)^2} + V^2 \cos^2 q_3 a}$$

where A – anharmonicity coefficient.

Bound states of optical phonons

- At $\varepsilon < 0$, bound states of phonons appear in the film for an arbitrarily small one A . Since the anharmonicity constant in the film is greater than in the bulk sample, the influence of the anharmonicity is greater and the levels corresponding to the bound states are located deeper. The matrix element oscillates depending on the film thickness L , and upon transition to a massive sample takes a maximum value A . As the film thickness $L = (N_3 + 1)a$ decreases, the bound state levels shift down. We estimated the value of the binding energy for *GaAs*, using the following values of physical quantities:

$$m^* = m_0 \sim 10^{-27} \text{ g}$$

$$d \sim 5 \cdot 10^{-7} \text{ cm (film thickness)}$$

$$\varepsilon_{0,|0|} \sim 5 \cdot 10^{-16} \text{ erg}$$

which is observable.



Conclusion

- ▶ For the case of two-dimensional free motion and one-dimensional quantization of the phonon energy spectrum, the existence of a new quasiparticle, which is a bound state of phonons, is proved. The features of the formation of bound states of phonons and the role of anharmonicity for such formation are discussed. Thus, a radical rearrangement of the phonon spectrum can occur in the case of phonon-phonon interaction with the formation of bound or resonance states of phonons in crystals. The obtained information can be used in modern phonon technologies to control the scattering frequency and dissipation rate of phonons in quantum devices: nanostructures and heterostructures [2].
- ▶ The values of carrier scattering frequencies on optical phonons in dimensionally limited structures exceed 10^{13} s^{-1} . These frequencies are among the highest in such structures. Therefore, such an interaction of carriers with phonons plays a major role in carrier mobility, which leads to a change in the laser gain.



References

- ▶ Csukanov A V and Kateev I. *J. Quantum Electronics* **48(7)** pp. 641-647. 2018.
- ▶ Строшило М., Дутта М. Фононы в наноструктурах. М. Физматлит, 320с. 2006.
- ▶ Wang CT, Wu ZY, Zhao CL, Ding ZH, Xiao IL *Chin.Phys. B* **21** 057108 . 2012.
- ▶ Davydov A. C. *Theory of a solid body* (M: Nauka) p. 647. 2010.