

International Workshop on Computational Nanotechnology

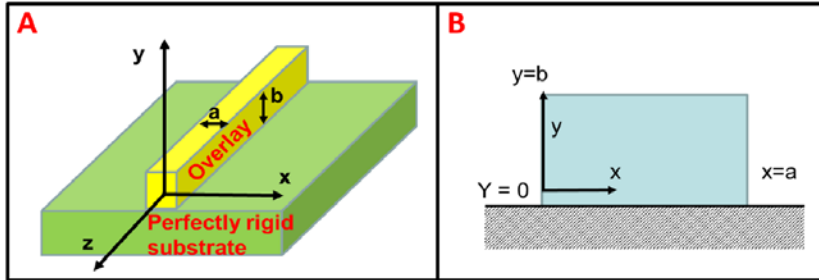


Figure 1: The 3D structure of the microsound waveguide is shown in the fig. A where overlay (yellow) part has much less rigidity compared to the substrate (green) hence substrate assumed to be perfectly rigid. The fig. B shows the rectangular cross-section of the waveguide which is the most common direction for implementing different waveguide structure.

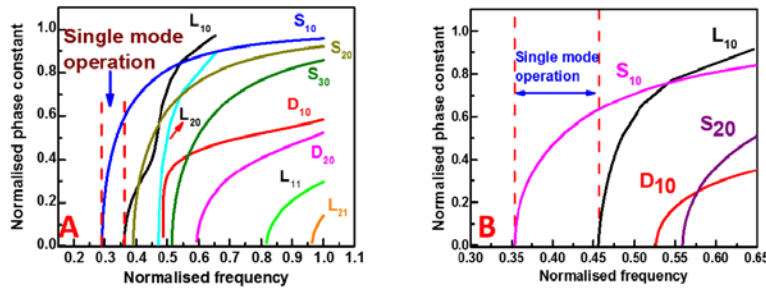


Figure 2: The dispersion curve for the A) $b/a = 0.3$ B) $b/a = 0.5$ ratio is given. The single mode operation window for both the ratio of height/width

- [1] Waldron, R.A., 1971. Mode spectrum of a microsound waveguide consisting of an isotropic rectangular overlay on a perfectly rigid substrate. IEEE Transactions on Sonics and Ultrasonics, 18(1), pp.8-15.
- [2] Stroschio, M.A. and Dutta, M., 2001. Phonons in Nanostructures. Cambridge University Press.

P:09 Effect of quantum confinement on lifetime of anharmonic decay of optical phonon in a confined GaAs structure

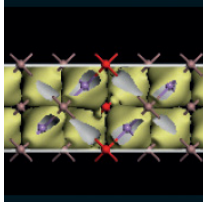
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In this research, the role of phonon confinement on the anharmonic decay of an LO is analyzed. Anharmonic interactions describe the decay of phonon modes in GaAs via the Klemens channel [1]. The interaction Hamiltonian for three phonon process can be written as [2] channel [1]. The interaction Hamiltonian for three phonon process can be written as [2]

$$H_{k,j;k',j';k'',j''} = \frac{1}{\sqrt{N}} P(k, j; k', j'; k'', j'') u_{k,j} u_{k',j'} u_{k'',j''} \quad (1)$$

where k, k', k'' are the three phonon wave vectors involved in the annihilation or creation process, j, j', j'' are the polarization of the three phonons and N = number of unit cells present. P describes the cubic (anharmonic) coupling. The phonon displacement in normal coordinates is represented as:



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$$u_{k,j} = \left(\frac{\hbar}{2m\omega_{k,j}} \right)^{\frac{1}{2}} e'_{k,j} (a_{k,j} e^{i\vec{k}\vec{r}} + a_{k,j}^{\dagger} e^{-i\vec{k}\vec{r}}) \quad (2a)$$

$$u(\vec{r}) = \frac{1}{\sqrt{N}} \sum_q \sum_{j=1,2,3} \left(\frac{\hbar}{2m\omega_{q,j}} \right)^{\frac{1}{2}} (a_{q,j} e^{i\vec{q}\vec{r}} \hat{e}_{q,j} + a_{q,j}^{\dagger} e^{-i\vec{q}\vec{r}} \hat{e}_{q,j}^*) = \frac{1}{\sqrt{N}} \sum_q \sum_{j=1,2,3} \overline{u_{q,j}} \quad (2b)$$

where $a_{k,j}$, $a_{k,j}^{\dagger}$ denoted the annihilation and creation operator, respectively, $e'_{k,j}$ is the polarization vector, m is the reduced mass of the lattice atoms and $\omega_{q,j}$, is the frequency of the normal mode. The displacement vector can be represented as following, with the direction of confinement and direction perpendicular to it [1].

$$u(\vec{r}) = e^{\pm i\vec{q}\vec{r}} = u(z) e^{\pm i\vec{q}_{\parallel}\vec{r}_{\parallel}} = (\cos(q_z z) \pm i \sin(q_z z)) e^{\pm i\vec{q}_{\parallel}\vec{r}_{\parallel}} \quad (3)$$

The decay lifetime for phonons can be calculated using Fermi golden rule, the matrix element in Fermi golden rule can be simplified as 1D problem for a quantum-confined structure confined in the z-direction.

$$\frac{1}{V} \int |M|^2_{ave} dV = \frac{1}{L_z} \int u^2(z) dz \quad (4)$$

Taking into account the confinement of the LO phonon in the GaAs structure to can be describe by either the slab model ($V = 0$ at $\pm L_z/2$) or the guided model ($u = 0$ at $\pm L_z/2$) [1] yields the same value for the average matrix element squared, respectively:

$$|M|^2_{ave} = \frac{1}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \sin^2 y dy = \frac{1}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos^2 y dy = \frac{1}{2} \quad (5)$$

These results indicate that the decay rate for the lowest LO phonon mode in either the slab or the guided model is approximately half that of the bulk phonon.

In this research, the confinement effect on the optical phonon decay lifetime in confined GaAs quantum structures is considered. This analysis is based on the three phonon interaction Hamiltonian; the phonon displacement vectors are defined in order to perform the calculation of the matrix element via the Fermi golden rule to estimate the lifetime for the Klemens channel in confined GaAs structures.

- [1] Strocio, M.A. and Dutta, M., 2001. *Phonons in Nanostructures*. Cambridge University Press.
- [2] Bhatt, A.R., Kim, K.W. and Strocio, M.A., 1994. Theoretical calculation of longitudinal-optical-phonon lifetime in GaAs. *Journal of Applied Physics*, 76(6), pp.3905-3907.