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Design of a Novel Heterostructure Photodetectors with Dramatically Enhanced Signal-to-Noise based on Resonant Interface-Phonon-Assisted Transitions and Engineering of Energy States to Enhance Transition Rates

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Optics-2014, 8-10 Sept. 2014

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A novel heterostructure photodetector design is presented that facilitates dramatic enhancements of signal-to-noise. The structure incorporates a single quantum well coupled to a symmetric double quantum well that makes it possible to engineer energy states with energy state separations equal to an interface phonon energy. In addition, quantum level energy degeneracy between states in the single-well and double-well systems makes it possible to enhance the rate of interface-phonon-assisted transitions. The techniques underlying this approach have been discussed previously by Stroscio and Dutta in Phonons in Nanostructures (Cambridge University Press, 2001). Together, these effects make it possible to greatly enhance signal-to-noise ratios in these heterostructure-based photodetectors. These designs are optimized based on Schrödinger equation calculations of the energy states and the determination of interface phonon potentials and dispersion modes by applying boundary conditions for which the phonon potential has corresponding continuous normal components of the displacement field and tangential components of electric fields. Novel photodetector designs with dramatically enhanced signal-to-noise will be presented for a number of different heterostructure devices.
This energy-level structure facilitates the absorption of a photon, emission of a phonon, and the absorption of a photon with the same wavelength as the original photon. $E_1$ is the first energy level of the single well, and $E_3$ is the second energy level. In addition, $E_2$, $E_2'$, $E_4$, and $E_4'$ represent the first, second, third, and forth energy levels for the double quantum well.

With reference to Fig. 1, it is straightforward to see that there will be a dramatic signal-to-noise enhancement in the current, $I_{sn,E1}$, from the deepest state $E_1$, relative to $I_{sn,E2}$, from the deepest state $E_2$ (without phonon-assisted transition and second photon absorption), as given by the Richardson formula:

$$\frac{I_{sn,E_1}}{I_{sn,E_2}} = e^{\frac{2E_{photon} - E_{phonon}}{kT}} = e^{\frac{E_{phonyon} - E_{phonon}}{kT}}$$

In this equation, $E_3 - E_1 = E_4' - E_2 = E_{photon}$ and $E_2' - E_2 = E_{phonon}$.

For example if, $\frac{E_{photon} - E_{phonon}}{kT} = 8$

a dramatic $1/3,000$ reduction can be realized.
Transverse Optical (TO) Phonon

Transverse Optical (TO) Phonon

Transverse Optical (TO) Phonon

Transverse Acoustic (TA) Phonon

LO and LA Phonons have displacements along the direction of q
Boundary Conditions:
Optical modes --- continuity of the tangential component of the electric field and the z component of the displacement vector must be continuous at the interfaces
Acoustic modes --- displacement and normal component of stress tensor are continuous at interfaces

For example
\[\varepsilon_{j,z} \frac{\partial \phi_j(z)}{\partial z} \bigg|_{z=z_j} = \varepsilon_{j+1,z} \frac{\partial \phi_{j+1}(z)}{\partial z} \bigg|_{z=z_j}\]

\[\omega^2 = C \left( \frac{1}{M_1} + \frac{1}{M_2} \right) \pm C \sqrt{\left( \frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2 \left( \frac{k\alpha}{2} \right)}{M_1 M_2}}\]

Quantized Confined Phonons
Normalization:
Mode amplitude normalized so that the energy in each model is the quantized phonon energy – example 2D graphene

\[ \frac{1}{S} \int_{s} (u \cdot u^* + v \cdot v^*) \, dx \, dy = \frac{\hbar}{2M \omega_{mn}^{LO}} \]
Elastic Continuum Theory Gives Correct Energy for a Dominant Mode of the Nanomechanical Modes in Carbon Nanotubes and in C\textsubscript{60}

McEwen & Park et al., Nature September 2000

Elastic Continuum Results

Mode Energy (meV)

- $a_0$: 62
- $a_1$: 74
- $a_2$: 111
- $b_2$: 32
- $b_3$: 38

35 meV mode observed experimentally

Matches our theoretical results to 10%

Goal: Theoretical Description of Nanoscale Mechanical Structures for Nanodevice and Sensor Applications including Nanocantilevers
Phonons: Some Basic Characteristics

Anharmonic Effects:
Klemen’s Channel with Keating Model ---Bhatt, Kim and Stroscio

Precision and Nature of Optical Phonon Confinement
H. Sakaki et al.

Figure 6.2: LO phonon lifetime in GaAs as a function of temperature. From Bhatt et al. (1994), American Institute of Physics, with permission.
Selection of Major Theoretical Papers: Optical Modes

- **K. J. Nash**, “Electron-Phonon Interactions and Lattice Dynamics of Optic Phonons in Semiconductor Heterostructures,” Physical Review, B46, 7723-7744 (1992). --- For slab modes, reformulated slab vibrations, and guided modes, “intrasubband and intersubband electron-phonon scattering rates are **independent of the basis set used to describe the modes, as long as this set is orthogonal and complete**.”
More on Confined, Interface, and Half-Space Phonon Modes in Phonons and Nanostructures
More on Interface Modes

\[ \varepsilon_1 \quad \varepsilon_2 \quad \varepsilon_1 \quad \varepsilon_2 \quad \varepsilon_1 \]

\[ -\frac{d_1}{2} - d_2 \quad -\frac{d_1}{2} \quad \frac{d_1}{2} \quad \frac{d_1}{2} + d_2 \]

\[ z = 0 \]
More on Interface Modes
More on Interface Modes
More on Interface Modes
Phonon “Bands”
Phonon “Bands”
Improved Semiconductor Lasers via Phonon-Assisted Transitions

Key Point -- Optical Devices not Electronic Devices!

Why? ENERGY SELECTIVITY

A single engineered phonon mode may be selected to modify a selected interaction
Interface Optical Phonons: Applications to Phonon-Assisted Transitions in Heterojunction Lasers
Interface-Phonon-Assisted Processes: Double Resonance Process

Gain enhancements greater than two orders of magnitude

Interface phonon modes dominate over bulk modes
Phonon enhanced inverse population in asymmetric double quantum wells

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New York 11794-3850

\[ \eta_{\text{tot}} = \frac{n_{A2}}{n_{A1}} = \frac{\tau_{21}}{\tau_{\text{out}}} \]

\[ = 6 \text{ for } a_1 = 8.5 \text{ nm} \]

\[ \eta_{\text{loc}} = \left( \frac{n_{A2}}{n_{A1}} \right)_k = 0 \]

\[ = \eta_{\text{tot}} \left( 1 + \frac{\tau_{11}}{\tau_{\text{out}}} \right)_{\text{EA2-A1/Ephonon}} \geq 50 - 100 \]
Phonon enhanced inverse population in asymmetric double quantum wells

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1. Model band diagram and energy levels of an AlAs/GaAs double quantum well heterostructure. Double-lined arrow corresponds to the light-emitting transition in the heterostructure. The inset shows the positions of three lowest subbands (in meV) as a function of the narrow well width $a_1$ (in nm) for fixed values $a_2=2$ nm and $a_3=10$ nm.

2. Onset for the interwell electron-phonon resonance. Solid line shows the total $A1\rightarrow B1$ transition rates by all confined and interface LO-phonon modes of a double-quantum well heterostructure as a function of the narrow well width $a_1$. Here $a_2=2$ nm and $a_3=10$ nm. Two dashed curves represent the interwell transition rates calculated in the single-mode bulk-like LO-phonon spectrum approximation with phonon energies: (a) $E_{LO}^{A1}=56$ meV, and (b) $E_{LO}^{A1}=51$ meV.

3. Peak values of the interwell optical-phonon-assisted transition rate under the double electron-phonon resonance condition. The curves are labeled with the value of the interwell transition width $a_1$ in nm. Figure 1 details individual contributions to the overall phonon-emission rate: dashed line-confined phonon modes, dotted line-interface phonon modes. Bold dashed line represents the rate of the nonresonative interwell intersubband transitions, $\tau_{out}^{-1}$, for the heterostructure with $a_1=18$ nm.

The exemplary intrawell $A2\rightarrow A1$ phonon-emission rate for the heterostructure with $a_1=18$ nm is shown in Fig. 3 by the bold dashed line. The total intersubband population ratio, $\eta_{tot}$, can be roughly estimated as $\eta_{tot}=\frac{\tau_{out}}{\tau_{in}+\tau_{out}}$ for the double resonance condition ($a_1=8.5$ nm) it is as high as $\eta_{tot}=5$. However, outside the resonance region the total population inversion disappears. Thus for $a_1=8.0$ nm, we have only $\eta_{tot}=0.5$. It is worth noting that the total subband populations determine the optical gain and the output power only in the high electron concentration limit. For low electron concentration $n_e=10^{17}$ cm$^{-2}$, the lasing action is governed by the non-equilibrium $k$-space population inversion between $A2$ and $A1$ subband bottoms which cannot be reduced to $\eta_{tot}$. In this case, the interwell depopulation rate becomes even more important. Assuming that $A2$ electrons are distributed in a narrow region near the subband bottom we have

$$\eta_{tot}^{-1} = \frac{\tau_{out}}{\tau_{in} + \tau_{out}} \approx \frac{1}{\tau_{in}} \frac{\tau_{out}}{\tau_{out}} = 1$$

For a large $A2\rightarrow A1$ separation and low values of $\tau_{out}$, the local population inversion can be significantly enhanced. For the double-quantum-well heterostructures with $a_1=8.5$ nm, $a_2=2$ nm, and $a_3=18$ nm, we find $\tau_{in}/\tau_{out}=0.6$ and $\Delta E_{A2/A1} = 52$ meV, which results in $\eta_{tot}=1/0.6$, and may be very favorable for the overall laser performance.

It should be clearly understood, however, that population inversion is not the only important parameter for a successful lasing design. For instance, one must be careful to minimize the leakage of electrons from the upper lasing level $A2$ through the third energy level $B3$ of the wide well. This can affect the useful injection current. In the process it has little effect on the population inversion but it increases the lasing threshold. For our exemplary heterostructure, calculations show that the level $B3$ can be located within less than one $k_B T$ from the level $A2$, thus suppressing phonon-assisted leakage by taking the active quantum well width $a_1 = 11.5$ nm and applying an external electric field $8$ kV/cm to satisfy the double electron-phonon resonance condition.
Double Resonance Scheme

ps transition rates

Interface-Phonon-Assisted Processes

References 4 and 5:


Figure 10.7. Energy dispersion curves for 60-Ångstrom-wide (solid lines) and 100-Ångstrom-wide (broken lines) Al$_{0.3}$Ga$_{0.7}$As/GaAs/Al$_{0.3}$Ga$_{0.7}$As quantum wells. Typical intersubband and intrasubband transitions are shown for both quantum wells. The energy gap for the GaAs well, $E_g$(GaAs), is taken as 1.4 eV and the ratio of the effective mass to the electron mass is taken as 0.067 for GaAs. From Kisin et al. (1997), American Institute of Physics, with permission.

----- 10 nm
_____ 6 nm

AlGaAs-GaAs-AlGaAs
x = 0.3
Interface-Phonon-Assisted Processes, Con’t

6 nm, RT

6 nm, RT, 10 meV

6 nm, RT, 60 meV
Interface-Phonon-Assisted Processes, Con’t

$\tau_{\text{out}} = 0.4 \text{ ps}$

$\tau_{\text{out}} = 0.6 \text{ ps}$

$\tau_{1-2} = 0.56 \text{ ps}$

--- all modes
--- w/o barrier
--- modes
A - 0.4 ps,
B - 0.5 ps,
C - 0.6 ps
Phonon Engineering: Some Key Techniques

- Dimensional Confinement and Boundary Effects Cause Plane Wave Phonons (Bulk Phonons) to be Replaced by Set of Modes --- Same as Putting Electromagnetic Wave in a Waveguide

- Bulk modes $\rightarrow$ Confined modes, plus interface modes, plus half-space modes with new energies, and spatial profiles.

SINCE CARRIER INTERACTIONS MUST CONSERVE ENERGY AND MOMENTUM HAVING NEW PHONON ENERGIES LEADS TO WAYS TO MODIFY CARRIER SCATTERING AND TRANSPORT...
**Phonon Engineering: Some Key Techniques**

**EXPLOITING THE FACT THAT NEW ENERGIES LEADS TO WAYS TO MODIFY CARRIER SCATTERING AND TRANSPORT ---**

- Phoron assisted transitions → Example: use to enhance population inversions in Quantum Cascade Lasers, Type-II Lasers, etc.

- Change phase space to modify interactions → In devices based on quantum wells, quantum wires, and quantum dots reduces the set of phonon momenta and energies allowed in transitions --- Example: Phase-space reductions in CNTs lead to enhanced carrier mobilities

- Modify materials to change phonons and thus interactions → Examples: (a) Form metal-semiconductor interface to eliminate selected interface modes; (b) Reduce carrier-phonon interactions through the design of In$_x$Ga$_{1-x}$N-based structures exhibiting one mode behavior

- Modify phonon lifetimes (by arranging for different anharmonic terms) and phonon speeds (by modifying dispersion relations)→ Reduce bottleneck effects; modify thermal transport

- Generate coherent phonons using Cerenkov effect (as an example) to amplify phonon effects
Some areas where phonon engineering has clear payoff:

improved gain in semiconductor lasers (especially lasers with narrow quantum wells like quantum cascade lasers),

enhance gain in Sb-lased lasers,

coherent phonon sources for non-charge-based binary switches and devices,

increasing carrier mobilities in CNTs,

improving CNT-based IR detectors based on understand phonon-assisted non-radiative recombination,

improving III-nitride-based device performance,

phonon engineering to modify thermal conductivity.
Abstract
Intersubband semiconductor lasers (ISLs) are of great interest for mid-infrared (2-20 micron) device applications. These semiconductor devices have a wide range of applications from pollution detection and industrial monitoring to military functions. ISLs have generally encountered several problems which include slow intrawell intersubband relaxation times due to the large momentum transfer and small wave-function overlap of the initial and final electron states in interwell transitions. Overall, the ISL's of the prior art are subject to weak intersubband population inversion. The semiconductor device of the present invention provides optimal intersubband population inversion by providing a double quantum well active region in the semiconductor device. This region allows for small momentum transfer in the intersubband electron-phonon resonance with the substantial wave-function overlap characteristic of the intersubband scattering.

Inventors: Belenky; Gregory (Port Jefferson, NY); Dutta; Mitra (Wilmette, IL); Kisin; Mikhail (Lake Grove, NY); Luryi; Serge (Setanket, NY); Stroscio; Michael (Wilmette, IL)
Assignee: The United States of America as represented by the Secretary of the Army (Washington, DC)
Resonant phonon-assisted depopulation in type-I and type-II intersubband laser heterostructures

M. V. Kisin\textsuperscript{1}, M. A. Stroscio\textsuperscript{2}, G. Belenky\textsuperscript{1}, and S. Luryi\textsuperscript{1}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure1.png}
\caption{Left: schematic band diagram of an asymmetric InAs/GaSb DQW modeling an active region of intersubband type-II cascade laser. Black arrow depicts the interband LO-phonon assisted depopulation process. Right: subband splitting in the upper part of the leaky window $\delta$. Short vertical arrows indicate the positions of the Van Hove singularities.}
\end{figure}

In conclusion, we show that in type-II intersubband laser heterostructures the interband LO-phonon-assisted scattering can be used as an efficient complementary process for the fast depopulation of the lower lasing states.

\textit{Inst. Phys. Conf. Ser. No 174: Section 5}

\textit{Paper presented at 29th Int. Symp. Compound Semiconductors, Lausanne, Switzerland, 7-10 October 2002}

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Phonon-Assisted Transitions in Heterostructure Lasers
Interface-Phonon-Assisted Processes: Double Resonance Process

References 1-9


B. S. Williams, B. Xu, Q. Hu, *Narrow-linewidth Terahertz Emission from Three-level Systems*, APL, 75, 2927 (1999); Refs. 2 and 5.


Implemented in QCL-like Heterostructure
Intersubband semiconductor lasers with enhanced subband depopulation rate

Abstract
Intersubband semiconductor lasers (ISLs) are of great interest for mid-infrared (2-20 micron) device applications. These semiconductor devices have a wide range of applications from pollution detection and industrial monitoring to military functions. ISLs have generally encountered several problems which include slow intrawell intersubband relaxation times due to the large momentum transfer and small wave-function overlap of the initial and final electron states in interwell transitions. Overall, the ISL's of the prior art are subject to weak intersubband population inversion. The semiconductor device of the present invention provides optimal intersubband population inversion by providing a double quantum well active region in the semiconductor device. This region allows for small momentum transfer in the intersubband electron-phonon resonance with the substantial wave-function overlap characteristic of the intersubband scattering.

Inventors: Belenky; Gregory (Port Jefferson, NY); Dutta; Mitra (Wilmette, IL); Kisin; Mikhail (Lake Grove, NY); Luryi; Serge (Setanket, NY); Stroscio; Michael (Wilmette, IL) Assignee: The United States of America as represented by the Secretary of the Army (Washington, DC) Appl. No.: 957531 Filed: September 21, 2001
Interface Phonon-assisted Transitions in Reduced Noise Single-Well--Double-Well Photodetectors
Design

$E_3 = E_2'$

$E_3 - E_1 = E_4' - E_2 = E_{\text{photon}}$

$E_2' - E_2 = E_{\text{phonon}}$

$E_1$ is the first energy level of the single well, and $E_3$ is the second energy level of it. At the meanwhile, $E_2$, $E_2'$, $E_4$, and $E_4'$ represent the first, second, third, and forth energy level for the double quantum well.
Phonon Potential

Let the phonon potentials ($\Phi$) for the given structure be defined as follow:

$$\begin{align*}
\Phi &= A e^{qz} & \text{when } z \leq 0 \\
\Phi &= B e^{qz} + C e^{-qz} & \text{when } 0 \leq z < d_1 \\
\Phi &= D e^{q(z-d_1)} + E e^{-q(z-d_1)} & \text{when } d_1 \leq z < d_2 \\
\Phi &= F e^{q(z-d_2)} + G e^{-q(z-d_2)} & \text{when } d_2 \leq z < d_3 \\
\Phi &= H e^{q(z-d_3)} + I e^{-q(z-d_3)} & \text{when } d_3 \leq z < d_4 \\
\Phi &= J e^{q(z-d_4)} + K e^{-q(z-d_4)} & \text{when } d_4 \leq z < d_5 \\
\Phi &= e^{-q(z-d_5)} & \text{when } z \geq d_5
\end{align*}$$

(1)

A, B, C, D, E, F, G H, I, J and K are constants in the potential equations.

At the heterointerface of region 1 and region 2, the dielectric function of the semiconductor in the structure under study is $\varepsilon$, then the following two condition have to be satisfied:

$$\Phi_1(Z) = \Phi_2(Z)$$

$$\varepsilon_1 \frac{\partial \Phi_1}{\partial z} = \varepsilon_2 \frac{\partial \Phi_2}{\partial z}$$

(2)
Phonon Potential

From the previous equations we can get the relationship between the constants:

\[
\begin{align*}
B &= \frac{A}{2} (1 - \frac{\varepsilon_1}{\varepsilon_2}) \\
C &= \frac{A}{2} (1 + \frac{\varepsilon_1}{\varepsilon_2}) \\
D &= \frac{1}{2} ((1 + \frac{\varepsilon_1}{\varepsilon_2}) B e^{q d_i} + (1 - \frac{\varepsilon_1}{\varepsilon_2}) C e^{-q d_i}) \\
E &= \frac{1}{2} ((1 - \frac{\varepsilon_1}{\varepsilon_2}) B e^{q d_i} + (1 + \frac{\varepsilon_1}{\varepsilon_2}) C e^{-q d_i}) \\
F &= \frac{1}{2} ((1 + \frac{\varepsilon_1}{\varepsilon_3}) D e^{q (d_2 - d_i)} + (1 - \frac{\varepsilon_1}{\varepsilon_3}) E e^{-q (d_2 - d_i)}) \\
G &= \frac{1}{2} ((1 - \frac{\varepsilon_1}{\varepsilon_3}) D e^{q (d_2 - d_i)} + (1 + \frac{\varepsilon_1}{\varepsilon_3}) E e^{-q (d_2 - d_i)})
\end{align*}
\]

And we can also get the secular equation of this system

\[
\frac{J e^{q (d_5 - d_4)} + K e^{-q (d_5 - d_4)}}{J e^{q (d_5 - d_4)} - K e^{-q (d_5 - d_4)}} = -\frac{\varepsilon_3}{\varepsilon_1}
\]

Plug the relationship between these constants into the secular equation we can then solve it to get the interface phonon modes of this system.
Phonon Potential

In order to calculate the potential of this system, we need to figure out the constants in the potential equations. So here we will normalize the potential of this system to get these constants.

For cubic material, the normalization condition is given by:

\[
\frac{\hbar}{2\omega L^2} = \sum_i \frac{1}{4\pi} \frac{1}{2\omega} \frac{\partial \epsilon_i(\omega)}{\partial \omega} \int_{R_i} dz (q^2 |\Phi_i(q, z)|^2 + \left| \frac{\partial \Phi_i(q, z)}{\partial z} \right|^2)
\] (5)

Then the normalization condition becomes:

\[
\frac{\partial \epsilon_1(\omega)}{\partial \omega} q A^2 + \frac{\partial \epsilon_2(\omega)}{\partial \omega} q (B^2 (e^{2qd_i} - 1) + C^2 (1 - e^{-2qd_i})) + \frac{\partial \epsilon_1(\omega)}{\partial \omega} q (D^2 (e^{2qd_i} - 1) + E^2 (1 - e^{-2qd_i}))
\]

\[
\frac{\partial \epsilon_3(\omega)}{\partial \omega} q (F^2 (e^{2q(d_3-d_2)} - 1) + G^2 (1 - e^{-2q(d_3-d_2)})) + \frac{\partial \epsilon_1(\omega)}{\partial \omega} q (H^2 (e^{2q(d_3-d_5)} - 1) + I^2 (1 - e^{-2q(d_3-d_5)}))
\]

\[
+ \frac{\partial \epsilon_3(\omega)}{\partial \omega} q (J^2 (e^{2q(d_5-d_4)} - 1) + K^2 (1 - e^{-2q(d_5-d_4)})) - \frac{\partial \epsilon_1(\omega)}{\partial \omega} q = \frac{4\pi \hbar}{L^2}
\] (6)

Plug the relationship between these constants into the normalization condition we can get a equation with one unknown \( A \), then we can solve it to get constant \( A \). As long as we know \( A \) we can calculate the rest constants.
Results

GaAlAs/GaAs material system

<table>
<thead>
<tr>
<th></th>
<th>GaAs</th>
<th>AlAs</th>
<th>Al_{x}Ga_{1-x}As</th>
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<tbody>
<tr>
<td>$\varepsilon_{\infty}$</td>
<td>10.89</td>
<td>8.16</td>
<td>10.89 - 2.73 $\times$ x</td>
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<tr>
<td>$\hbar \omega_{\text{LO}}$ (GaAs-like) (meV)</td>
<td>36.25</td>
<td>...</td>
<td>36.25 - 6.55$\times$ x + 1.79$\times$x^2</td>
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<td>$\hbar \omega_{\text{TO}}$ (GaAs-like) (meV)</td>
<td>33.29</td>
<td>...</td>
<td>33.29 - 0.64$\times$ x - 1.16$\times$x^2</td>
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<tr>
<td>$\hbar \omega_{\text{LO}}$ (AlAs-like) (meV)</td>
<td>...</td>
<td>50.09</td>
<td>44.63 + 8.78$\times$ x - 3.32$\times$x^2</td>
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<tr>
<td>$\hbar \omega_{\text{TO}}$ (AlAs-like) (meV)</td>
<td>...</td>
<td>44.88</td>
<td>44.63 + 0.55$\times$ x - 0.30$\times$x^2</td>
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We calculate the parameters we need

<table>
<thead>
<tr>
<th>Phonon modes</th>
<th>Ga_{0.452}Al_{0.548}As (AlAs-like)</th>
<th>GaAs</th>
<th>Ga_{0.741}Al_{0.259}As (GaAs-like)</th>
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<tr>
<td>LO</td>
<td>48.44</td>
<td>36.25</td>
<td>34.67</td>
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<tr>
<td>TO</td>
<td>44.83</td>
<td>33.29</td>
<td>33.046</td>
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Results

Interfaces phonon modes at $q=1e8$ (wavevector)

<table>
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<td>33.38808</td>
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<tr>
<td>33.8125</td>
<td>44.9045</td>
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<tr>
<td>34.193</td>
<td>46.278</td>
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<tr>
<td>34.6304</td>
<td>47.1212</td>
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<tr>
<td>35.57657</td>
<td>48.038603</td>
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</tbody>
</table>
Dispersion curve
Phonon Potential
Phonon Potential

Potential (meV/nm) vs. nm

Phonon Potential

Potential (meV/nm) vs. nm

33.8125 meV

33.38808 meV

34.193 meV

34.6304 meV

34.6304 meV
Phonon Potential

Potential (meV nm)

nm

47.1212 meV
44.9045 meV
35.57657 meV
46.278 meV
Results

InGaAs/InAs material system

For In$_x$Ga$_{1-x}$As

<table>
<thead>
<tr>
<th>InAs-like</th>
<th>GaAs-like</th>
</tr>
</thead>
<tbody>
<tr>
<td>242.99 − 32.54$x + 4.545x^2$</td>
<td>TO</td>
</tr>
<tr>
<td>253.97 − 67.91$x + 51.94x^2$</td>
<td>LO</td>
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Then, we calculate the parameters we need

<table>
<thead>
<tr>
<th>Phonon modes (meV)</th>
<th>$\text{In}<em>{0.248}\text{Ga}</em>{0.752}\text{As}$</th>
<th>$\text{In}<em>{0.59}\text{Ga}</em>{0.41}\text{As}$</th>
<th>InAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO</td>
<td>35.32</td>
<td>28.746</td>
<td>29.74</td>
</tr>
<tr>
<td>TO</td>
<td>32.89</td>
<td>27.93</td>
<td>27.01</td>
</tr>
<tr>
<td>$\varepsilon_\infty$</td>
<td>11.526</td>
<td>11.287</td>
<td>11.7</td>
</tr>
</tbody>
</table>
Results

Interfaces phonon modes at \( q=1e8 \) (wavevector)

<table>
<thead>
<tr>
<th>IF Phonon modes (meV)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>29.542</td>
<td>33.6199006</td>
</tr>
<tr>
<td>30.351</td>
<td>34.72185</td>
</tr>
<tr>
<td>32.7285</td>
<td>35.1522</td>
</tr>
</tbody>
</table>
Results

29.542 meV
34.72185 meV
35.1522 meV
33.6199006 meV
32.7285 meV
30.351 meV
Results

InAlAs/InP material system

For $\text{In}_x\text{Al}_{1-x}\text{As}$

<table>
<thead>
<tr>
<th>Phonon modes (meV)</th>
<th>$\text{In}<em>{0.36}\text{Al}</em>{0.64}\text{As}$</th>
<th>InP</th>
<th>$\text{In}<em>{0.61}\text{Al}</em>{0.39}\text{As}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LO</td>
<td>46.977</td>
<td>42.75</td>
<td>29.16</td>
</tr>
<tr>
<td>TO</td>
<td>43.57</td>
<td>37.63</td>
<td>29.23</td>
</tr>
<tr>
<td>$\varepsilon_\infty$</td>
<td>9.4344</td>
<td>9.61</td>
<td>10.32</td>
</tr>
</tbody>
</table>
Results

Interfaces phonon modes
at q=1e8 (wavevector)

<table>
<thead>
<tr>
<th>IF Phonon modes (meV)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>29.18687</td>
<td>44.314</td>
</tr>
<tr>
<td>38.383165</td>
<td>45.15</td>
</tr>
<tr>
<td>40.99825</td>
<td>45.8385</td>
</tr>
<tr>
<td>43.679</td>
<td></td>
</tr>
</tbody>
</table>
GaAs/Ga\textsubscript{1-x}Al\textsubscript{x}As

- Band Gap, \( E_g = (1.426 + 1.247x) \) eV
- Band alignment: 33\% of total discontinuity in valence band, i.e. \( \Delta V_{VB} = 0.33 \); \( \Delta V_{CB} = 0.67 \)
- Electron effective mass, \( m^* = (0.067 + 0.083x)m_0 \)

\textit{From Quantum Wells, Wires and Dots (Paul Harrison)}

\begin{itemize}
  \item \( dE_{g1} = 1.247 \times x \times 0.67 \)
  \item \( dE_{g2} = 1.247 \times y \times 0.67 \)
  \item \( m^*_{Ga_{1-x}Al_xAs} = 0.067 + 0.083 \times x \)
  \item \( m^*_y_{GaAs} = 0.067 \)
  \item \( m^*_{Ga_{1-y}Al_yAs} = 0.067 + 0.083 \times y \)
\end{itemize}
InGaAs Design

In\textsubscript{1-x-y}Al\textsubscript{x}Ga\textsubscript{y}As/Al\textsubscript{As}

- Total band discontinuity,
  \[ \Delta V = \left[ 2.093x + 0.629y + 0.577x^2 + 0.436y^2 + 1.013xy - 2.0x^2(1 - x - y) \right] \]
- Band alignment: 47\% of total discontinuity in valence band, i.e.
  \( \Delta V_{VB} = 0.47; \Delta V_{CB} = 0.53 \)
- Electron effective mass, \( m^* = (0.0427 + 0.0685x)m_0 \)

For In\textsubscript{1-y}Ga\textsubscript{y}As/Al\textsubscript{As},
\[ \Delta V = [(0.629y + 0.436y^2) \times 0.53] \text{ eV in conduction band} \]
Effective mass =, \( m^* = (0.0427)m_0 \)
\[ dE_{g1} = (0.0629y_1 + 0.436y_1^2) \times 0.53 \]
\[ dE_{g2} = (0.0629y_2 + 0.436y_2^2) \times 0.53 \]
\[ m_{In_{1-y_1}Ga_{y_1}As}^* = 0.0427 \]
\[ m_{InAs}^* = 0.0427 \]
\[ m_{In_{1-y_v}Ga_{y_v}As}^* = 0.0427 \]
InAlAs/InP Design

In_{1-x-y}Al_{x}Ga_{y}As/AlAs

- **Total band discontinuity,**
  \[ \Delta V = [2.093x + 0.629y + 0.577x^2 + 0.436y^2 + 1.013xy - 2.0x^2(1 - x - y)] \text{ eV} \]
- **Band alignment:** 47% of total discontinuity in valence band,
  i.e. \( \Delta V_{VB} = 0.47; \Delta V_{CB} = 0.53 \)
- **Electron effective mass,** \( m^* = (0.0427 + 0.0685x)m_0 \)

*From Quantum Wells, Wires and Dots (Paul Harrison)*

For In_{1-x}Al_{x}As/AlAs,
\[ \Delta V = [(2.093x - 1.423x^2 + 2x^3) \times 0.53] \text{ eV in conduction band} \]

Effective mass\( =, m^* = (0.0427 + 0.0685x)m_0 \)


FIG. 1. Calculated valence-band offsets are combined with measured low-temperature band gaps to yield the energy band diagram (in eV) for the heterointerfaces in the In_{0.53}Ga_{0.47}As/In_{0.53}Al_{0.47}As/InP(001) family.
\[ \text{d}E_g_1 = (2.093x_1 - 1.423x_1^2 + 2x_1^3) \times 0.53 - 0.135921 \]
\[ \text{d}E_g_2 = (2.093x_1 - 1.423x_1^2 + 2x_1^3) \times 0.53 - 0.135921 \]
\[ m_{In_{1-x_1}Al_{x_1}As}^* = 0.0427 + 0.0685x_1 \]
\[ m_{InP}^* = 0.08 \]
\[ m_{In_{1-x_2}Al_{x_2}As}^* = 0.0427 + 0.0685x_2 \]
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