Solid State Physics Part II

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- II-1. Lattice vibrations (10/29)
- II-2. Electronic States (11/05)
- II-3. Energy Bands (11/12)
- II-4. Lattice Thermal Properties (11/19)
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Lattice Vibrations

1. Harmonic Approximation

2. Vibration of crystal with monatomic basis

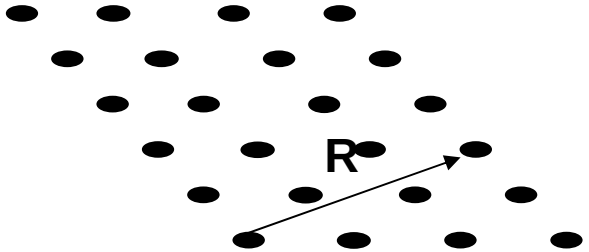
3. Two atoms per primitive cell

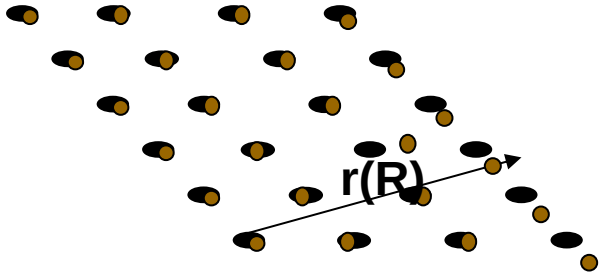
4. Phonons in Superlattices

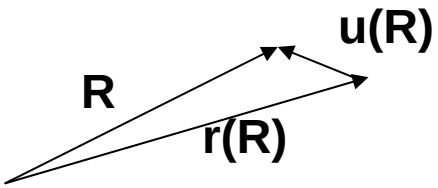
HW assignment: Ch. 6, Problems 5, 6, and 8.

1. Harmonic approximation

- The lattice of points, specified by vectors **R**.
- A particular instantaneous configuration of ions. The ion whose mean position is **R** is found at **r**(**R**)
- If **u**(**R**)= **r**(**R**)-**R** is small, we can approximate the potential
- U(**r-R**) by ½ K (**r-R**)^2 = ½ K **u**^{2} …… harmonic approximation





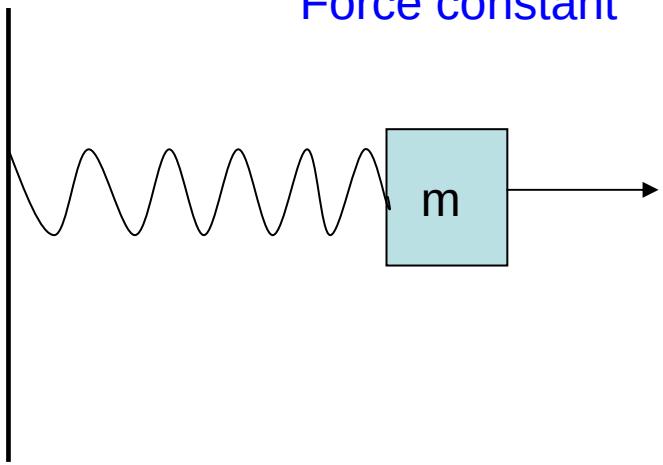


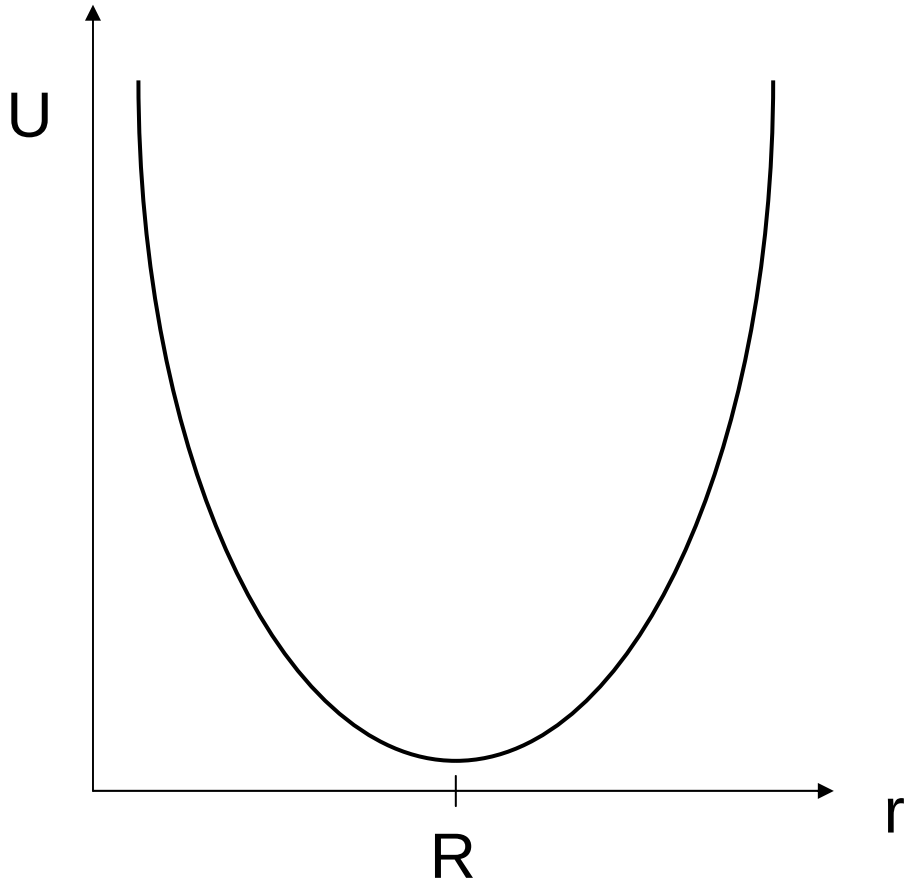
Simple Harmonic Motion

$$U(r-R) = \tfrac{1}{2}K\,(r-R)^2$$

$$F = -\,\partial U/\partial r = -K\,u$$

Force constant

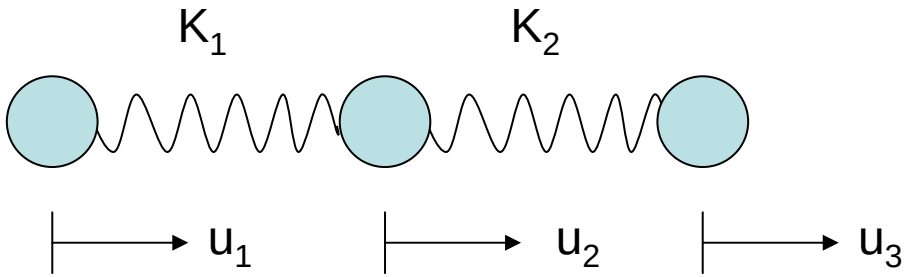




$F = ma = m\ddot{u} = -K\,u$

$u(t) = A\cos(\omega t)$; $\omega^2 = K/m$

Three coupled oscillators



$$m\frac{d^2u_1}{dt^2} = -K_1(u_1 - u_2), \qquad (6\text{-}1)$$

$$m\frac{d^2u_2}{dt^2} = -K_1(u_2 - u_1) - K_2(u_2 - u_3), \qquad (6\text{-}2)$$

$$m\frac{d^2u_3}{dt^2} = -K_2(u_3 - u_2), \qquad (6\text{-}3)$$

Solving coupled equations

Replace ü by $-\omega^2 u$ everywhere

$$(K_1 - m\omega^2)u_1 - K_1u_2 = 0, \qquad (6\text{-}4)$$

$$-K_1u_1 + (K_1 + K_2 - m\omega^2)u_2 - K_2u_3 = 0, \qquad (6\text{-}5)$$

$$-K_2u_2 + (K_2 - m\omega^2)u_3 = 0, \qquad (6\text{-}6)$$

Rearrange into an eigen-value equation

$$\begin{vmatrix} K_1 & -K_1 & 0 \\ -K_1 & K_1+K_2 & -K_2 \\ 0 & -K_2 & K_2 \end{vmatrix} \begin{vmatrix} u_1 \\ u_2 \\ u_3 \end{vmatrix} = m\omega^2 \begin{vmatrix} u_1 \\ u_2 \\ u_3 \end{vmatrix}$$

Solution

Eigen-values:

$$\omega_1 = 0, \qquad \text{(Pure translational motion)} \tag{6-9}$$

$$\omega_2 = \frac{1}{m}\left[(K_1 + K_2) - (K_1^2 + K_2^2 - K_1K_2)^{1/2}\right]^{1/2}, \tag{6-10}$$

$$\omega_3 = \frac{1}{m}\left[(K_1 + K_2) + (K_1^2 + K_2^2 - K_1K_2)^{1/2}\right]^{1/2}. \tag{6-11}$$

Δ

Eigen-vectors: (with an arbitray scaling factor)

$u_2=1,\ u_1=K_1/(K_1-m\ \omega^2),\ \ u_3=K_2/(K_2-m\ \omega^2)$

e.g. $K_1=1$, $K_2=3$

$\Delta=2.65$

For mode 2:

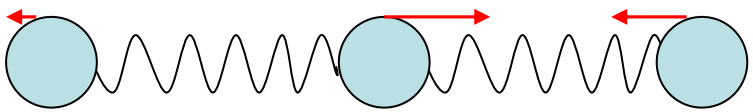
$u_1= - K_1/(K_2+\Delta)$ $\quad u_3= - K_2/(K_1+\Delta)$

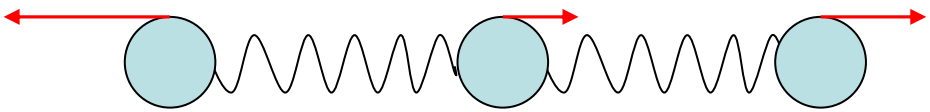
$= -1/5.65$ $\quad = - 3/3.65$

For mode 3:

$u_1 = - K_1/(K_2- \Delta)$ $\quad u_3= K_2/(\Delta -K_1)$

$= - 1/0.35$ $\quad = 3/1.65$

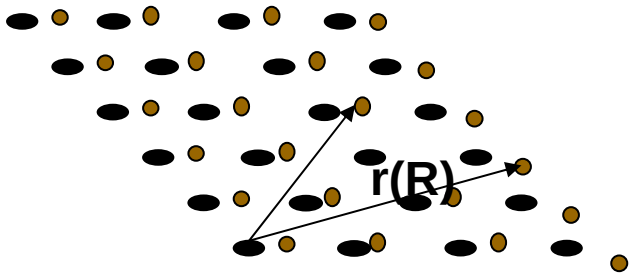




Crystal potential

- Potential $$U = \frac{1}{2}\sum_{R,R'} \phi(r(R) - r(R')) = \frac{1}{2}\sum_{R,R'} \phi(R - R' + u(R) - u(R'))$$

$$f(r+a) = f(r) + a\cdot\nabla f(r) + \frac{1}{2}(a\cdot\nabla)^2 f(r) + \frac{1}{3!}(a\cdot\nabla)^3 f(r) + \ldots$$



$$U = U^{eq} + U^{harm}$$

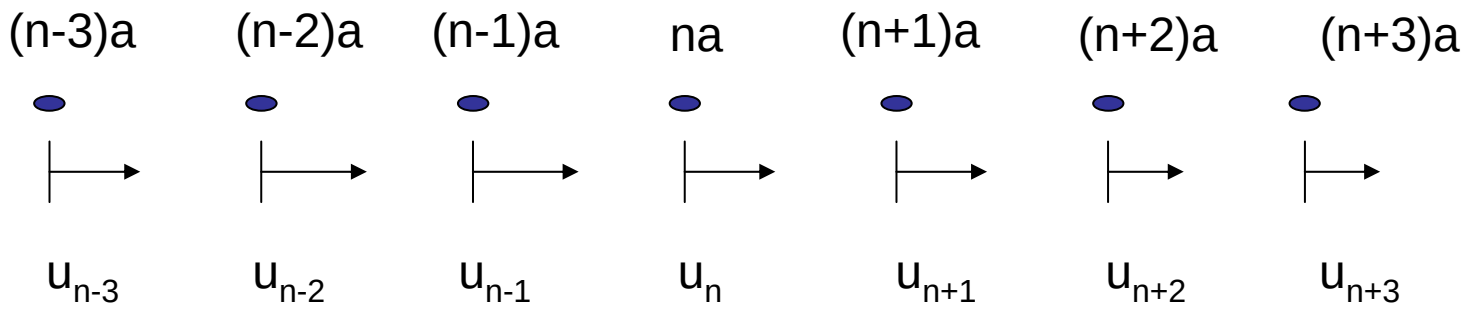
$$U^{harm} = \frac{1}{4}\sum_{\substack{R,R' \\ \mu,\nu=x,y,z}} [u_\mu(R) - u_\mu(R')]\phi_{\mu\nu}(R - R')[u_\nu(R) - u_\nu(R')]$$

$$\phi_{\mu,\nu} = \frac{\partial^2 \phi(r)}{\partial r_\mu \partial r_\nu}$$

$$= \tfrac{1}{2} \sum_{\mu\,\nu} \Phi_{\mu\,\nu} u_\mu u_\nu$$

$$F_\mu = \sum_{\mu\,\nu} \Phi_{\mu\,\nu} u_\nu$$

2. Normal modes of a one dimensional monatomic lattice



$U = \frac{1}{2} K \sum_n (u_{n+1}-u_n)^2$

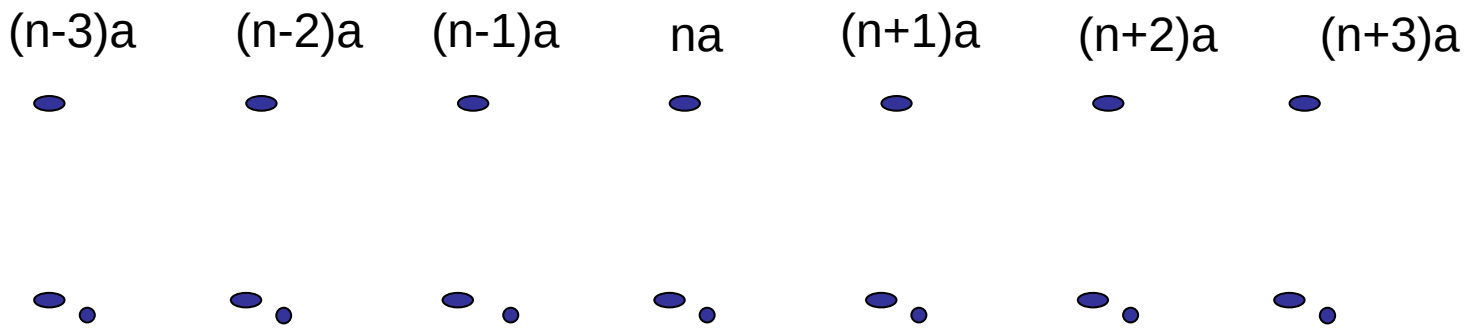
$F_n = K(u_{n+1}-u_n)+K(u_{n-1}-u_n) = m\ddot{u}_n = - m \omega^2 u_n$

Bloch theorem: $u_{n+s} = e^{iksa} u_n$

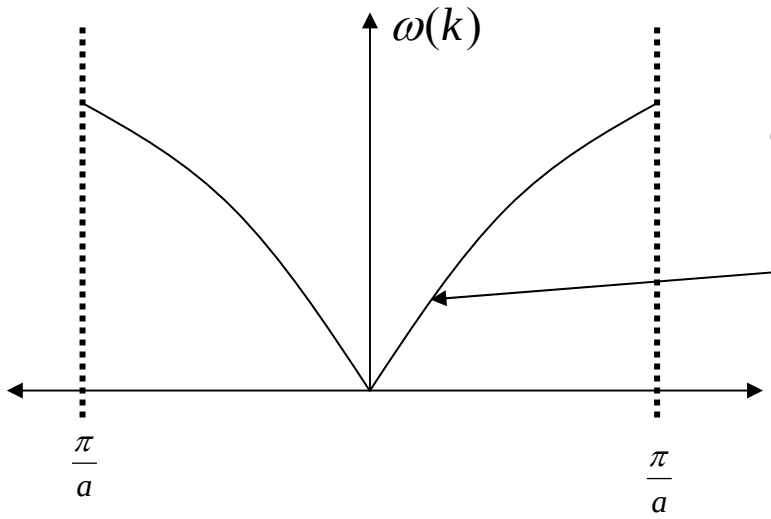
So, $u_{n \pm 1} = e^{\pm ika} u_n$

Thus, $-m\omega^2 u_n = K [e^{ika}+e^{-ika} -2] u_n = 2K [\cos(ka)-1] u_n$

Dispersion relation of a one dimensional monatomic lattice



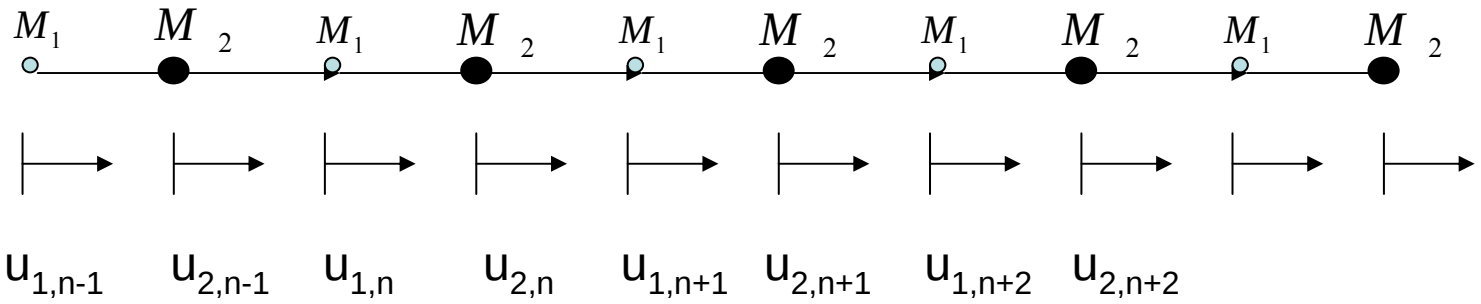
Acoustical branch



$$\omega(k) = 2\sqrt{\frac{K}{M}}\left|\sin\left(\frac{1}{2}ka\right)\right|$$

$$= \sqrt{\frac{K}{M}}\,ka \quad for \quad ka \to 0$$

3. Two ions per primitive cell



$$F_{1,n} = K\,(u_{2,n}-u_{1,n}) + K\,(u_{2,n-1}-u_{1,n}) = -\,m_1\,\omega^2\,u_{1,n}$$

$$F_{2,n} = K\,(u_{1,n+1}-u_{2,n}) + K\,(u_{1,n}-u_{2,n}) = -\,M_2\,\omega^2\,u_{2,n}$$

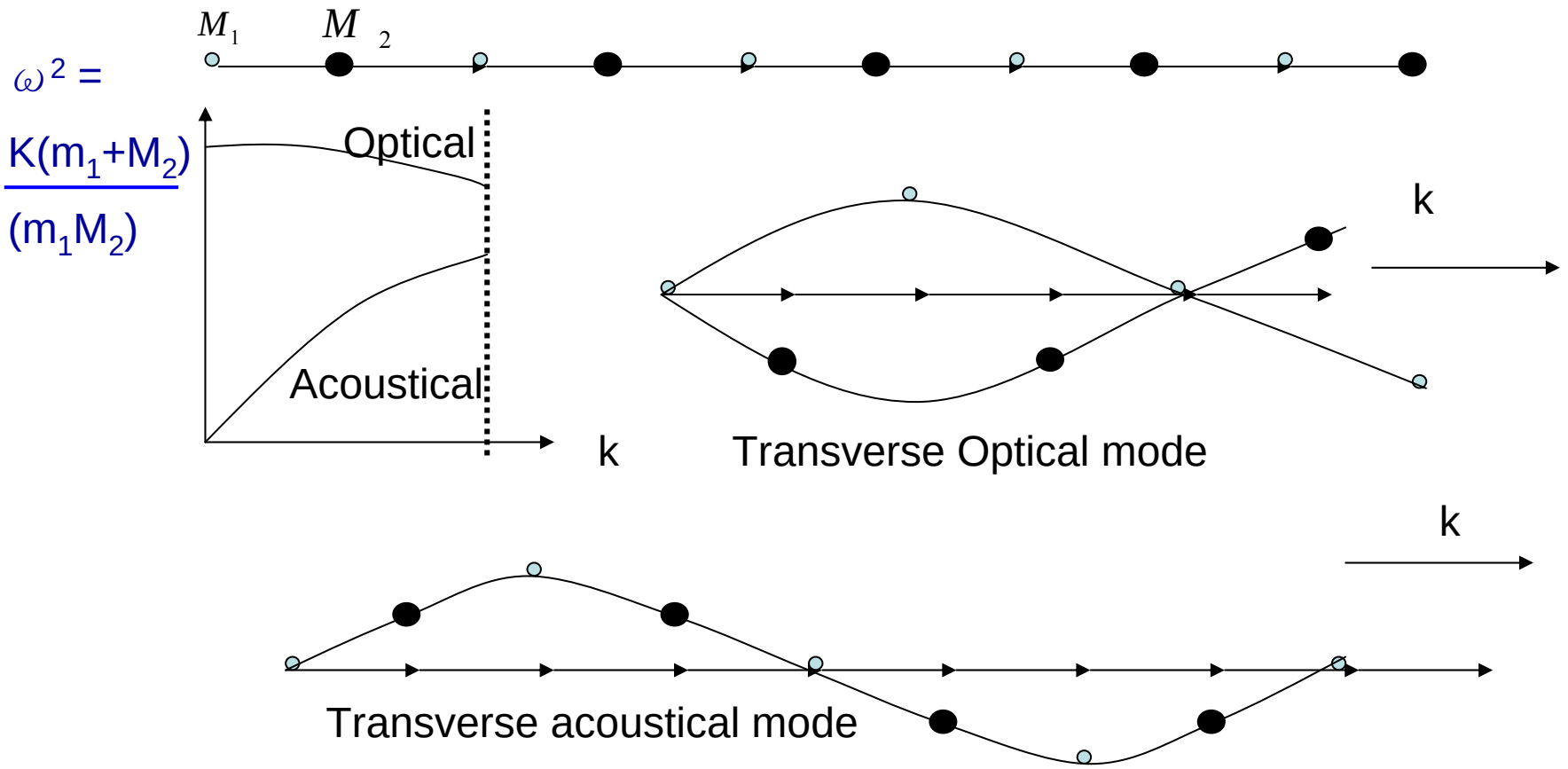
$$K\,(u_{2,n} - u_{1,n}) + K\,(u_{2,n}\,e^{-iqa} - u_{1,n}) = -\,m_1\,\omega^2\,u_{1,n}$$
$$K\,(u_{1,n}\,e^{iqa} - u_{2,n}) + K\,(u_{1,n} - u_{2,n}) = -\,M_2\,\omega^2\,u_{2,n}$$

$$\begin{vmatrix} 2K-m_1\,\omega^2 & -K(1+e^{-iqa}) \\ -K(e^{iqa}+1) & 2K-m_2\,\omega^2 \end{vmatrix} = 0$$

Solutin for two ions per primitive cell

$(2K-m_1\omega^2)(2K-M_2\omega^2)-4K^2\cos^2(\frac{1}{2}qa)=0$

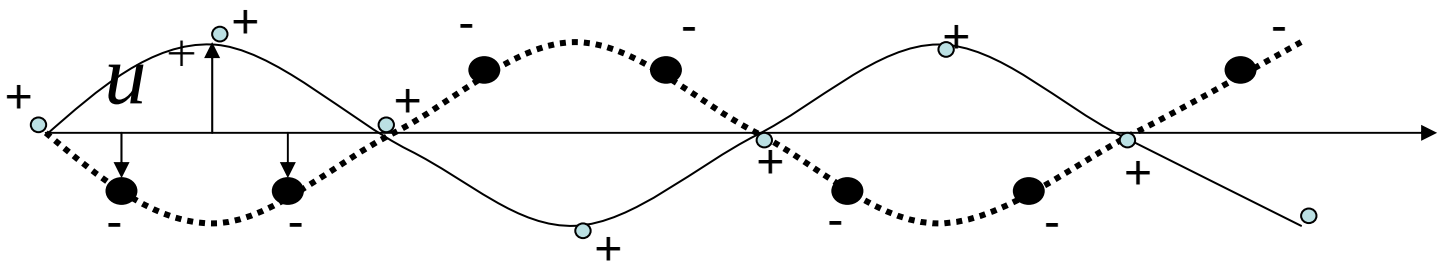
$\omega^2 = K(m_1+M_2)/(m_1M_2) \pm K\,[(m_1+M_2)^2/(m_1M_2)^2-4\sin^2(\frac{1}{2}qa)/m_1M_2\,]^{\frac{1}{2}}$



Optical mode

- Because the long wavelength optical modes in ionic crystals can interact with electromagnetic radiation, and are responsible for much of the characteristic optical behavior of such crystal

$$\vec{D} = \varepsilon \vec{E} + 4\pi \vec{P}$$



- The oppositely charged ions in each primitive cell undergo oscillate against each other, giving rise to a non vanishing polarization density

Interaction with electromagnetic field

- Dipole moment of the primitive cell
- The displacement of the positive and negative ions satisfy equations

$$P = eW, \qquad W = u^{+} - u^{-}$$

$$M_{+}\frac{\partial^2 u^{+}}{\partial t^2} = -K(u^{+} - u^{-}) + eE^{L}$$

$$M_{-}\frac{\partial^2 u^{-}}{\partial t^2} = -K(u^{-} - u^{+}) - eE^{L}$$

- ,which can be written

$$\frac{\partial^2 W}{\partial t^2} = \frac{e}{M}E^{L} - \frac{K}{M}W$$

- Where M is the ionic reduced mass, $M^{-1} = (M_{+})^{-1} + (M_{-})^{-1}$
- Fo r $E^{L} = \mathrm{Re}(E_0 e^{-i\omega t},)$ we obtain

$$W = \mathrm{Re}(W_0 e^{-i\omega t}); W_0 = \frac{eE_0 / M}{\omega^2 - \omega^2}$$

$10^{-1}\,to \quad 10^{-2}\,eV$

Lattice vibrations in 3D crystals

Let $\mathbf{R}_\alpha = \mathbf{R}^0_\alpha + \mathbf{u}^\alpha$. Tayler expand inter-atomic potential $U(\{\mathbf{R}\})$ around $\{\mathbf{R}_0\}$:

$$U(\{\mathbf{R}\}) = E_n(\{\mathbf{R}\}) + \frac{1}{2}\sum_{\alpha\alpha'} \mathbf{u}^{(\alpha)} \cdot \mathbf{D} \cdot \mathbf{u}^{(\alpha')},$$

$$D_{ij}(\mathbf{R}^0_\alpha, \mathbf{R}^{\prime 0}_\alpha) = \frac{\partial^2 U}{\partial u_i^{(\alpha)} \partial u_j^{(\alpha')}}.$$

Use translational invariance:

$$U(\{\mathbf{R}_\alpha + \mathbf{R}_1\}) = U(\{\mathbf{R}_\alpha\})$$

$$\Rightarrow D_{ij}(\mathbf{R}_\alpha + \mathbf{R}_1, \mathbf{R}^0_{\alpha'} + \mathbf{R}_1) = D_{ij}(\mathbf{R}^0_\alpha, \mathbf{R}^0_{\alpha'}) \text{ for any } \mathbf{R}_1$$

$$\text{So, } D_{ij}(\mathbf{R}^0_{\alpha'}, \mathbf{R}^0_{\alpha'}) = D_{ij}(\mathbf{R}^0_\alpha - \mathbf{R}^0_{\alpha'}, 0) = D_{ij}(\mathbf{R}^0_\alpha - \mathbf{R}^0_{\alpha'})$$

Normal-mode transformation:

We expect the normal mode solution to take the form

$$\mathbf{u}^{(\alpha)} = \frac{1}{\sqrt{MN}} Re[\hat{\epsilon}_\lambda(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{R}^0_\alpha}]$$

$$\text{Define } \mathbf{D}(\mathbf{k}) = \frac{1}{M}\sum_\alpha \mathbf{D}(\mathbf{R}^0_\alpha) e^{-i\mathbf{k}\cdot\mathbf{R}^0_\alpha} \cdots \text{ dynamic matrix}$$

$$\text{NOTE: } \mathbf{D}(\mathbf{k}) = \mathbf{D}(\mathbf{k}+\mathbf{G}),\ \mathbf{D}^*(\mathbf{k}) = \mathbf{D}(-\mathbf{k}),\ D(\mathbf{k}) = D^+(\mathbf{k}).$$

$$\text{where } \mathbf{D}(\mathbf{k}) \cdot \hat{\epsilon}_\lambda(\mathbf{k}) = \omega^2_\lambda(\mathbf{k}) \hat{\epsilon}_\lambda(\mathbf{k});\ \lambda = 1, 2, 3$$

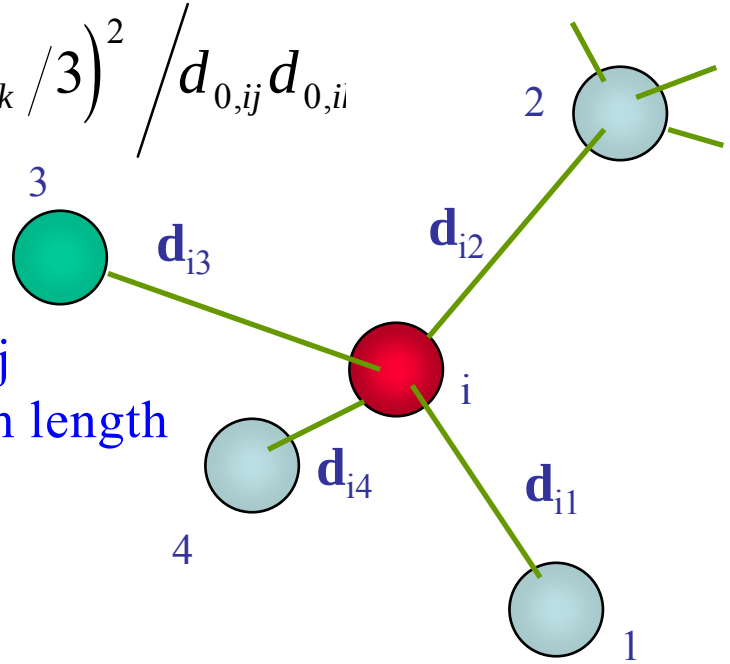
ω_λ=normal mode frequency. $\hat{\epsilon}_\lambda$= polarization vector .

Valence force field (VFF) Model

$$V = \frac{1}{4}\sum_{ij}\frac{3}{4}\alpha_{ij}\left(d_{ij}^2 - d_{0,ij}^2\right)^2 \Big/ d_{0,ij}^2$$

$$+\frac{1}{4}\sum_{i}\sum_{j\neq k}\frac{3}{4}\beta_{ijk}\left(\vec{d}_{ij}\cdot\vec{d}_{ik} + d_{0,ij}d_{0,ik}/3\right)^2 \Big/ d_{0,ij}d_{0,ik}$$

i labels atom positions
j , k label nearest-neighbors of i
d_{ij} = bond length joining sites i and j
$d_{0,ij}$ is the corresponding equilibrium length
α_{ij}= bond stretching constants
d_{ijk}= bond bending constants
We take $d_{ijk}^2 = d_{ij}d_{ik}$



Theory of Elasticity

After distortion, the lattice vectors become

$$\mathbf{R}' = \mathbf{R} + \mathbf{u}(\mathbf{r}) = (n_1 + u_x)\hat{x} + (n_2 + u_y)\hat{y} + (n_3 + u_z)\hat{z} \equiv n_1\hat{x}' + n_2\hat{y}' + n_3\hat{z}',$$

where $\hat{x}'$, $\hat{y}'$, $\hat{z}'$ are primitive lattice vectors for the distorted lattice. We define

$$\hat{x}' = (1 + \epsilon_{xx})\hat{x} + \epsilon_{xy}\hat{y} + \epsilon_{xz}\hat{z},\ \ \hat{y}' = \epsilon_{yx}\hat{y} + (1 + \epsilon_{yy})\hat{y} + \epsilon_{yz}\hat{z}$$

$$\hat{z}' = \epsilon_{zx}\hat{y}x + \epsilon_{zy}\hat{y} + (1 + \epsilon_{zz})\hat{z}.$$

$$\text{Thus} \begin{cases} u_x = n_1\epsilon_{xx} + n_2\epsilon_{yx} + n_3\epsilon_{zx} \\ u_y = n_1\epsilon_{xy} + n_2\epsilon_{yy} + n_3\epsilon_{zy} \\ u_z = n_1\epsilon_{xz} + n_2\epsilon_{yz} + n_3\epsilon_{zz} \end{cases}$$

In the continuum limit $(n_1, n_2, n_3) \to (x, y, z)$ and we obtain $\epsilon_{ji} = (\frac{\partial u_i}{\partial r_j})$.

The strain tensor (e_{ij}) is defined as $e_{ij} = e_{ji} = \hat{x}'_i \cdot \hat{x}_j - \delta_{ij}$.

$$\text{So,} \begin{cases} e_{xx} = \epsilon_{xx} = \frac{\partial u_x}{\partial x} \\ e_{yy} = \epsilon_{yy} = \frac{\partial u_y}{\partial y} \\ e_{zz} = \epsilon_{zz} = \frac{\partial u_z}{\partial z} \end{cases}$$

$$\begin{cases} e_{xy} = \epsilon_{yz}(1 + \epsilon_{xx}) + \epsilon_{xy}(1 + \epsilon_{yy}) + \epsilon_{xz}\epsilon_{yz} \approx \epsilon_{yx} + \epsilon_{xy} \\ e_{yy} = \epsilon_{yz} + \epsilon_{zy} \\ e_{zx} = \epsilon_{zx} + \epsilon_{xz} \end{cases}$$

Strain tensor :

$e_{\alpha\ \beta} = \partial u_{\alpha} / \partial x_{\beta} + \partial u_{\beta} / \partial x_{\alpha}$ if $\alpha \neq \beta$

$e_{\alpha\ \alpha} = \partial u_{\alpha} / \partial x_{\alpha}$

$$\text{Dilation} = \text{fractional increase in volume}$$

$$\Delta = \frac{V' - V}{V} = e_{xx} + e_{yy} + e_{zz} \ldots \text{ hydrostatic component}$$

$$(pf)\ V = \hat{x} \cdot (\hat{y} \times \hat{z}) = 1 \text{ (in units of } a^3)$$

$$V' = \hat{x}' \cdot (\hat{y}' \times \hat{z}') = \begin{Vmatrix} 1 + \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yz} & 1 + \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & 1 + \epsilon_{zz} \end{Vmatrix}$$

$$\approx 1 + e_{xx} + e_{yy} + e_{zz}.$$

Stress & Strain

⋆ Stress: (force per unit area)

$\mathcal{T}_{ij} = i$-th component of force per unit area acting on a surface with normal direction $\|\hat{x}_j$

The stress must be applied such that the net torque and net force are zero (so the solid remains at rest)

$\mathcal{T}_{ij} = \mathcal{T}_{ji}$, is a symmetric tensor.

So, we only need six components,$\alpha = xx, yy, zz, yz, zx, xy$.

⋆ Hooke's Law: For small deformation, the strain is linearly proportional to the stress:

$$e_\alpha = \sum_\beta \mathcal{S}_{\alpha\beta}\mathcal{T}_\beta \equiv \mathcal{S}_{\alpha\beta}\mathcal{T}_\beta$$

(the sum over repeated subscripts is implied)

$\mathcal{S}_{\alpha\beta}$ is called the compliance tensor.

The inverse of the above gives

$$\mathcal{T}_\alpha = \sum_\beta \mathcal{C}_{\alpha\beta}e_\beta,$$

where $\mathcal{C}_{\alpha\beta}$ is called the elastic (stiffness) constants.

Elastic energy density

Define $U = \frac{1}{2}\sum_{\alpha\beta}\tilde{\mathcal{C}}_{\alpha\beta}e_\alpha e_\beta$ to be the elastic energy per unit volume.

$$\mathcal{T}_\mu = \frac{\partial}{\partial e_\mu} = \frac{1}{2}\sum_{\alpha\beta}\tilde{\mathcal{C}}_{\alpha\beta}(\delta_{\alpha\mu}e_\beta + e_\alpha\delta_{\beta\mu}) = \frac{1}{2}\sum_{\beta}(\tilde{\mathcal{C}}_{\mu\beta} + \tilde{\mathcal{C}}_{\beta\mu})e_\beta = \sum_{\beta}\mathcal{C}_{\beta\mu}\ e_\beta$$

Thus the elastic constant tensor is also symmetric.

$$\Rightarrow U = \frac{1}{2}\sum_{\alpha\beta}\mathcal{C}_{\alpha\beta}e_\alpha e_\beta = \frac{1}{2}\sum_{\alpha}\mathcal{T}_\alpha e_\alpha.$$

⋆Example: For cubic crystals, x, y, z directions are equivalent.

So, we have $C_{11} = C_{22} = C_{22}, C_{12} = C_{13} = C_{23}, C_{44} = C_{55} = C_{66}$.

$$U = \frac{1}{2}\sum_{\alpha\beta}\mathcal{C}_{\alpha\beta}e_\alpha e_\beta = \frac{1}{2}[C_{11}(e_{xx}^2 + e_{yy}^2 + e_{zz}^2) + C_{44}(e_{yx}^2 + e_{zx}^2 + e_{xy}^2)] + C_{12}(e_{yy}e_{zz} + e_{zz}e_{xx} + e_{xx}e_{yy}).$$

Terms like $e_{xx}e_{xy}$, $e_{yz}e_{zx}$, $e_{xx}e_{yz}$ vanish, since they are invariant under 4-fold rotations, i.e.

$$C_{14} = C_{15} = C_{16} = c_{45} = C_{46} = C_{56} = 0.$$

$\star$ Strain stress table

	e_{xx}	e_{yy}	e_{zz}	e_{yz}	e_{zx}	e_{xy}
$\mathcal{T}_{xx}$	C_{11}	C_{12}	C_{12}	0	0	0
$\mathcal{T}_{yy}$	C_{12}	C_{11}	C_{12}	0	0	0
$\mathcal{T}_{zz}$	C_{21}	C_{21}	C_{11}	0	0	0
$\mathcal{T}_{yz}$	0	0	0	C_{44}	0	0
$\mathcal{T}_{xz}$	0	0	0	0	C_{44}	0
$\mathcal{T}_{xy}$	0	0	0	0	0	C_{44}

Inverting the matrix, we have

$$S_{44} = C_{44}^{-1}, (S_{11} - S_{12}) = (C_{11} - c_{12})^{-1}, (S_{11} + 2S_{12}) = (C_{11} + 2C_{12})$$

Elastic wave equation

$\star$ Bulk modulus, $B = -VdP/dV$

For hydrostatic strain, $e_{xx} = e_{yy} = e_{zz} = \frac{1}{3}\delta$ (uniform dilation)

$e_{xy} = e_{yz} = e_{xz} = 0$ (no shear strain)

$$U = \frac{3}{2}(C_{11} + 2C_{12})e_{xx}^2 = \frac{1}{6}(C_{11} + 2C_{12})\delta^2$$

$$\frac{\Delta V}{V} = e_{xx} + e_{yy} + e_{zz} = \delta$$

$$B = (dV/d\delta)/\delta = \frac{1}{3}(C_{11} + 2C_{12}) = 1/K,$$

where $K = -\frac{dV}{dP}\frac{1}{v}$ is called compressibility.

$\star$ Elastic wave equation:

$$\rho\frac{\partial^2 u_x}{\partial t^2} = \frac{\partial}{\partial x}\mathcal{T}_{xx} + \frac{\partial}{\partial y}\mathcal{T}_{xy} + \frac{\partial}{\partial z}\mathcal{T}_{xz}$$

$$\text{or } \rho\frac{\partial^2 u_i}{\partial t^2} = \sum_j(\partial\mathcal{T}_{ij}/\partial x_j)(\rho = \text{ mass density})$$

$$= C_{11}\frac{\partial e_{xx}}{\partial x} + C_{12}(\frac{\partial e_{yy}}{\partial x} + \frac{\partial e_{zz}}{\partial_x}) + C_{44}(\frac{\partial e_{xy}}{\partial y} + \frac{\partial e_{zx}}{\partial z}).$$

Sound velocity

Since $e_{ij} = \partial u_j / \partial x_i$, we have

$$\rho \frac{\partial u_x^2}{\partial t^2} = C_{11} \frac{\partial^2 u_x}{\partial x^2} + C_{44} \left(\frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial y^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 u_y}{\partial x \partial y} + \frac{\partial u_z^2}{\partial x \partial z} \right).$$

The permutation $(x \to y, x \to z)$ gives two other equations for u_y and u_z.

$\star$[100] propagation:

$u_x = u_0 e^{i(kx - \omega t)}$ (a trial solution)

$\Rightarrow \omega^2 \rho = -C_{11} k^2$

$v_l = \omega / k = \sqrt{C_{11}/\rho} =$ sound velocity of longitudinal wave.

Try $u_x = v_0 e^{i(ky - \omega t)}$ (a transverse wave or shear wave)

$\Rightarrow \omega^2 \rho = -C_{44} k^2 \Rightarrow v_t = \omega / k = \sqrt{C_{44}/\rho} =$ sound velocity of transverse wave

Rigid-ion model for 3D crystals

• Rigid-ion model (RIM) for phonons:

Consider a zincblende crystal. Each unit cell has two ions with effective charges $-Q$ and Q. Assume that the electronic cloud moves rigidly with the ions.

NOTE: This is different from adiabatic approximation, since the electron charge density $|\phi(\{\mathbf{r}\},\{\mathbf{R}\})|^2$ around ions should be deformed as ions move. We wish to solve the equation of motion

$$\sum_{\sigma' j'} D^{\sigma\sigma'}_{kk'}(\mathbf{k})\epsilon^{(\sigma')}_{j'} = M_\sigma \omega^2(\mathbf{k})\epsilon^{(\sigma)}_j;\ \sigma = 1,2;\ j = x,y,z,$$

$$\text{where}\ \ D^{\sigma\sigma'}_{jj'}(\mathbf{k}) = \sum_{\mathbf{R}} D^{\sigma\sigma'}_{jj'}(\mathbf{R}+\mathbf{S}_\sigma-\mathbf{S}_{\sigma'})e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{S}_\sigma-\mathbf{S}_{\sigma'})}.$$

$\mathbf{R}$ = lattice vectors, $\mathbf{S}_\sigma(\sigma = 1,2)$ = position vectors of ions within the unit cell, and

$$D^{\sigma\sigma}_{jj'}(\mathbf{R}+\mathbf{S}_\sigma-\mathbf{S}_{\sigma'}) = \frac{\partial^2 U}{\partial u^{(\sigma)}_j(\mathbf{R})\partial u^{(\sigma')}_{j'}(\mathbf{0})}$$

Short-range & Long-range interaction

U is the inter-atomic potential.

$$\text{*NOTE: } D^{\sigma' \sigma}_{j' j}(\mathbf{R} + \mathbf{S}_\sigma - \mathbf{S}_{\sigma'}) = D^{\sigma \sigma'}_{j j'}(-\mathbf{R} - \mathbf{S}_\sigma + \mathbf{S}_{\sigma'}).$$

The inter-atomic potential includes electron-ion interaction and the ion-ion interaction, screened by the valence electrons

$$\text{Thus, } U = U_{SR} + U_C,$$

$$\text{where } U_C = -{\sum_{\alpha\alpha'}}' \frac{Q^2}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|};\ Q = \text{ effective charge-transfer}$$

U_{SR} = short-range correction. Similarly, $D = D_{SR} + D_C$ (dynamic matrix). The columb term can be calculated exactly, whereas the short-range term is treated empirically. Symmetry can be used to reduce the number of empirical parameters.

Example: An eleven-parameter RIM for zincblende crystals [K. Kunc et al. Phys Status Solidi B72, 229(1975)].

The short-range term is trunctated at the second neighbors:

(i) nearest-neighbor term: $\mathbf{S} = (1,1,1), (1,-1,-1), (-1,1,-1), (-1,-1,1)$ (in units of $a/4$).

For $\mathbf{S} = (111)$

$$D^{12}(\mathbf{S}) = D^{21}(-\mathbf{S}) = \begin{pmatrix} A & B & B \\ B & A & B \\ B & B & A \end{pmatrix}.$$

(ii) 2nd-neighbor term: $\mathbf{R} = (\pm 2, \pm 2, 0), (\pm 2, 0, \pm 2), (0, \pm 2, \pm 2)$. For $\mathbf{R} = (2, 2, 0)$

$$D^{\sigma\sigma}\mathbf{R} = [D^{\sigma\sigma}(-\mathbf{R})]^t = \begin{pmatrix} C_\sigma & D_\sigma & E_\sigma \\ D_\sigma & C_\sigma & E_\sigma \\ -E_\sigma & -E_\sigma & F_\sigma \end{pmatrix}; \ \sigma = 1, 2.$$

*NOTE: The harmonic energy

$$U^{harm} = \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}', \sigma\sigma'} \mathbf{u}^{(\sigma)}(\mathbf{R}) \cdot \mathbf{D}^{\sigma\sigma'}(\mathbf{R} + \mathbf{S}_\sigma - \mathbf{R}' - \mathbf{S}_{\sigma'}) \cdot \mathbf{u}^{(\sigma')}(\mathbf{R}').$$

The net force exerted on an atom at $(\mathbf{R} + \mathbf{S}_\sigma)$ is

$$\sum_{\mathbf{R}'\sigma'} \mathbf{D}^{\sigma\sigma'}(\mathbf{R} + \mathbf{S}_\sigma - \mathbf{R}' - \mathbf{S}_{\sigma'}) \cdot \mathbf{u}^{(\sigma')}(\mathbf{R}'),$$

which vanishes if $\mathbf{u}^{(\sigma')}(\mathbf{R}') = \mathbf{d}$.

$$\Rightarrow \sum_{\mathbf{R}\sigma'} \mathbf{D}^{\sigma\sigma'}(\mathbf{R} + \mathbf{S}_\sigma - \mathbf{S}_{\sigma'}) = 0.$$

$$\text{So,} \quad D^{11}(0) + \sum_{\mathbf{S}}{}' D^{12}(\mathbf{S}) + \sum_{\mathbf{R}} D^{11}(\mathbf{R}) = 0$$

$$D^{22}(0) + \sum_{\mathbf{S}} D^{21}(-\mathbf{S}) + \sum_{\mathbf{R}} D^{22}(\mathbf{R}) = 0$$

$$\Rightarrow \mathbf{D}^{\sigma\sigma'}(0) = -4(A_\sigma + 2C_\sigma + F_\sigma)\mathbf{1}.$$

Examples of phonon bands

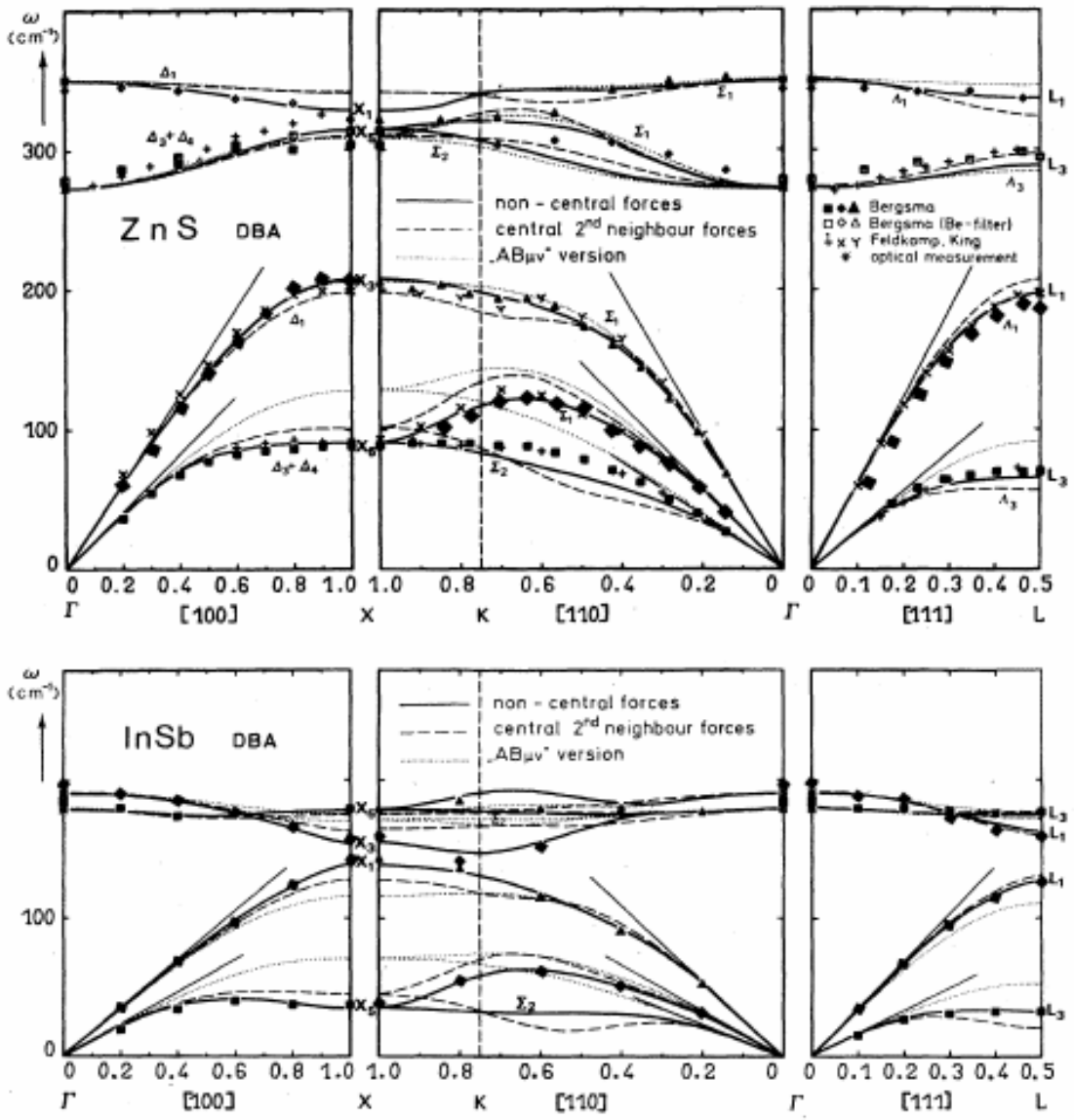


FIG. 1. Dispersion curves of ZnS and InSb calculated using the 15-parameter version of the DDM (solid lines) compared to neutron and optical measurements of phonon frequencies (Refs. 29(a) and 31–35 for ZnS, and Ref. 36 for InSb). Various stages in the process of determination of parameters lead to simplified models which are represented by broken and dotted lines (second-neighbor central forces and central springs, respectively). The results of similar calculations for ZnSe, GaP, GaAs, SiC, CuCl, and CuI are given in Ref 4.

Kunc & Balkanski, Phys. Rev. B **12**, 4346 (1975)

Performing the Ewald sum

*NOTE: The Coulomb term contains a summation of alternating series which converges extremely slowly. Any truncation of the sum at finite $|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|$ can lead to error due to boundary terms. To overcome this difficulty, one can use the Ewald's method.

• Ewald's method for evaluating the Coulumb term:
Write $V(\mathbf{r}) = \frac{1}{r}$ as the sum of a fast-decayng and a slow-decaying term,

$$V(\mathbf{r}) = V_F(\mathbf{r}) + V_s(\mathbf{r})$$

where $V_F(r) = \frac{1}{r} erfc(\alpha r)$ and $V_S(r) = \frac{1}{r} erf(\alpha r)$,

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt = 1 - erfc(x).$$

α is an adjustable parameter.

$$\text{Define } \phi(\mathbf{k}, \mathbf{r}) = \sum_{\mathbf{R}} (\mathbf{r} + \mathbf{R}) e^{i\mathbf{k}\cdot\mathbf{R}} = \frac{1}{v} \sum_{\mathbf{G}} \tilde{V}(\mathbf{G} + \mathbf{k}) e^{-i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}},$$

where $\tilde{V}(\mathbf{k}) = \int d^3r V(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$, v = unit cell volume. So,

$$\phi(\mathbf{k}, \mathbf{r}) = \frac{1}{v} \sum_{\mathbf{G}} \tilde{V}_S(\mathbf{G}, \mathbf{k}) e^{-i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}} + \sum_{\mathbf{R}} V_F(\mathbf{r} + \mathbf{R}) e^{i\mathbf{k}\cdot\mathbf{R}}$$

$$\text{Note: } \tilde{V}_S(\mathbf{k}) = \frac{4\pi}{k^2} e^{-k^2/4\alpha^2} \text{ is fast-decaying in } \mathbf{k}\text{-space.}$$

$$D_{jj'}^{\sigma\sigma'}(\mathbf{k}) = \frac{\partial^2}{\partial r_j \partial r_{j'}} \phi(\mathbf{k}, \mathbf{r})|_{\mathbf{r}=\mathbf{S}_\sigma - \mathbf{S}_{\sigma'}}.$$

$$= Q_\sigma Q_{\sigma'} [\frac{1}{v} \sum_G \tilde{V}_S(\mathbf{G}+\mathbf{k})(\mathbf{G}+\mathbf{k})_j \cdot (\mathbf{G}+\mathbf{k})_{j'} e^{-i(\mathbf{G}+\mathbf{k})\cdot(\mathbf{S}_\sigma - \mathbf{S}_{\sigma'})} + \sum_{\mathbf{R}}{}' H_{jj'}(\mathbf{R}+\mathbf{S}_\sigma - \mathbf{S}_{\sigma'}) e^{i\mathbf{k}\cdot\mathbf{R}}],$$

where

$$H_{jj'}(\mathbf{r}) = \frac{\partial^2}{\partial r_j \partial r_{j'}} V_F(\mathbf{r}) = \frac{3 r_j r_{j'} - \delta_{jj'} r^2}{r^5} erfc(\alpha r) - \frac{2\alpha}{\sqrt{\pi} r^2} e^{\alpha r^2} [\delta_{jj'} - \frac{r_j r_{j'}}{r^2}(2\alpha^2 r^2 + 3)].$$

*NOTE: The self-interaction term must be excluded. In the real-space sum of V, we must exclude the term $\mathbf{R} = 0$. This is indicated by $\sum'_{\mathbf{R}}$ in the fast-decaying term. For the slow-decaying term, we simply subtract $\frac{\partial^2}{\partial r_j \partial r_{j'}} V_S(\mathbf{r})|_{\mathbf{r}=0}$.

$$\text{For } \; r \to 0, V_S(\mathbf{r}) = \frac{2}{\sqrt{\pi} r} \int_0^{\alpha r} [1 - t'] dt = \frac{2\alpha}{\sqrt{\pi}} = \frac{2\alpha^2 r^2}{3\sqrt{\pi}}$$

$$\Rightarrow \frac{\partial^2}{\partial r_j \partial r_{j'}} V_S(\mathbf{r})|_0 = -\frac{4\alpha^2}{3\sqrt{\pi}} \delta_{jj'}.$$

Concept of Phonons

⋆ Phonons: quantization of lattice vibration

1. Energy of a vibrational mode (normal mode) with frequency ω is $E = (n + 1/2)\hbar\omega$, which corresponds to the creation of n quanta(phonons). The ground state ($n = 0$, or zero phonon) has an energy $\frac{1}{2}\hbar\omega$ (zero-point motion).

2. Phonon is particle-like, and it has a momentum $\hbar\mathbf{k}$ (k restricted in the 1st Brillouin zone) Because $\mathbf{k}$ and $\mathbf{k}' = \mathbf{k} + \mathbf{G}$ are equivalent, we call the momentum the "crystal momentum".

3. Phonons are bosons, so more than one phonon can occupy the same mode.

Average occupancy:

$$n(\eta\omega) = \frac{1}{e^{\frac{\eta\omega}{k_B T}} - 1}$$

Netron scattering from Phonons

Typically $\mathbf{G} = 0$ (normal process) has the largest contribution and $\mathbf{G} \neq 0$ (umklapp process) are less important.

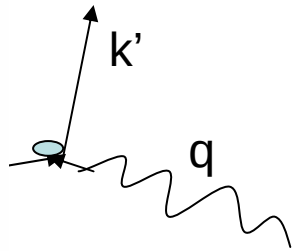
Use the energy conservation :

$$\frac{\hbar^2 k^2}{2M_n} = \frac{\hbar^2 k'^2}{2M_n} \pm \hbar\omega.$$

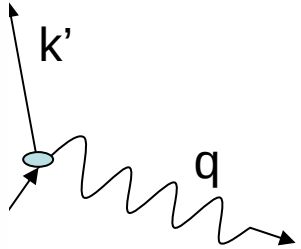
Measuring the energy ($\sim k'^2$) of the scattered neutron as a function of scattered angle θ, where

$$k^2 + k'^2 - 2kk' \cos\theta = q^2$$

allows one to determine ω versus $\mathbf{q}$.



absorption



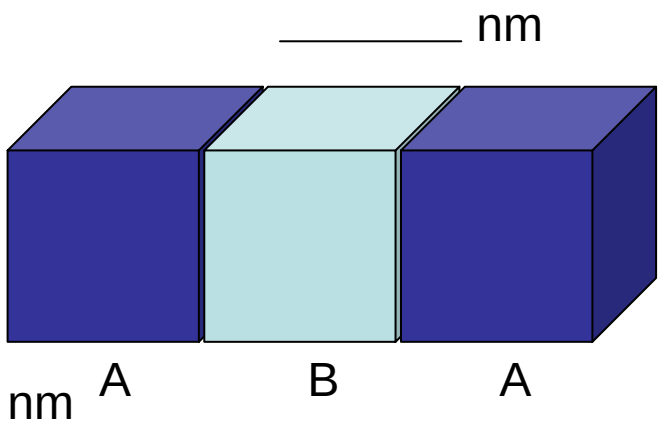
emission

- Phonon excitation is the main reason that resistivity of metal, alloy, and semiconductor occurs at room temperature.

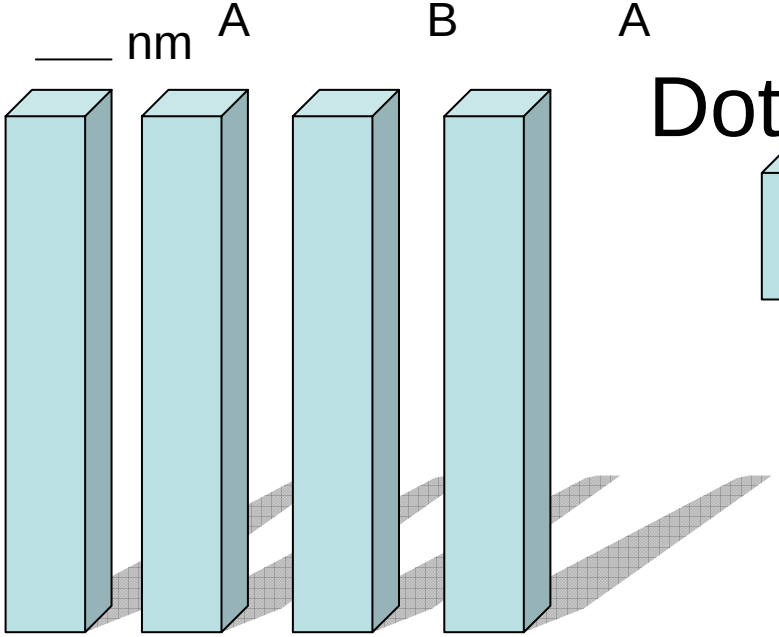
$$k' = k \pm q$$

Well, Wire and Dot

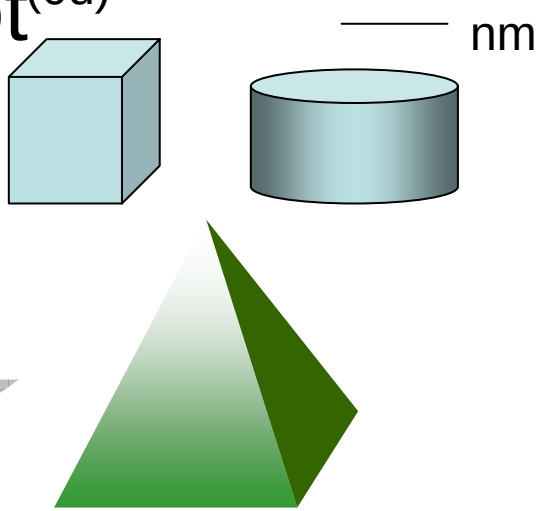
- Well (2d)



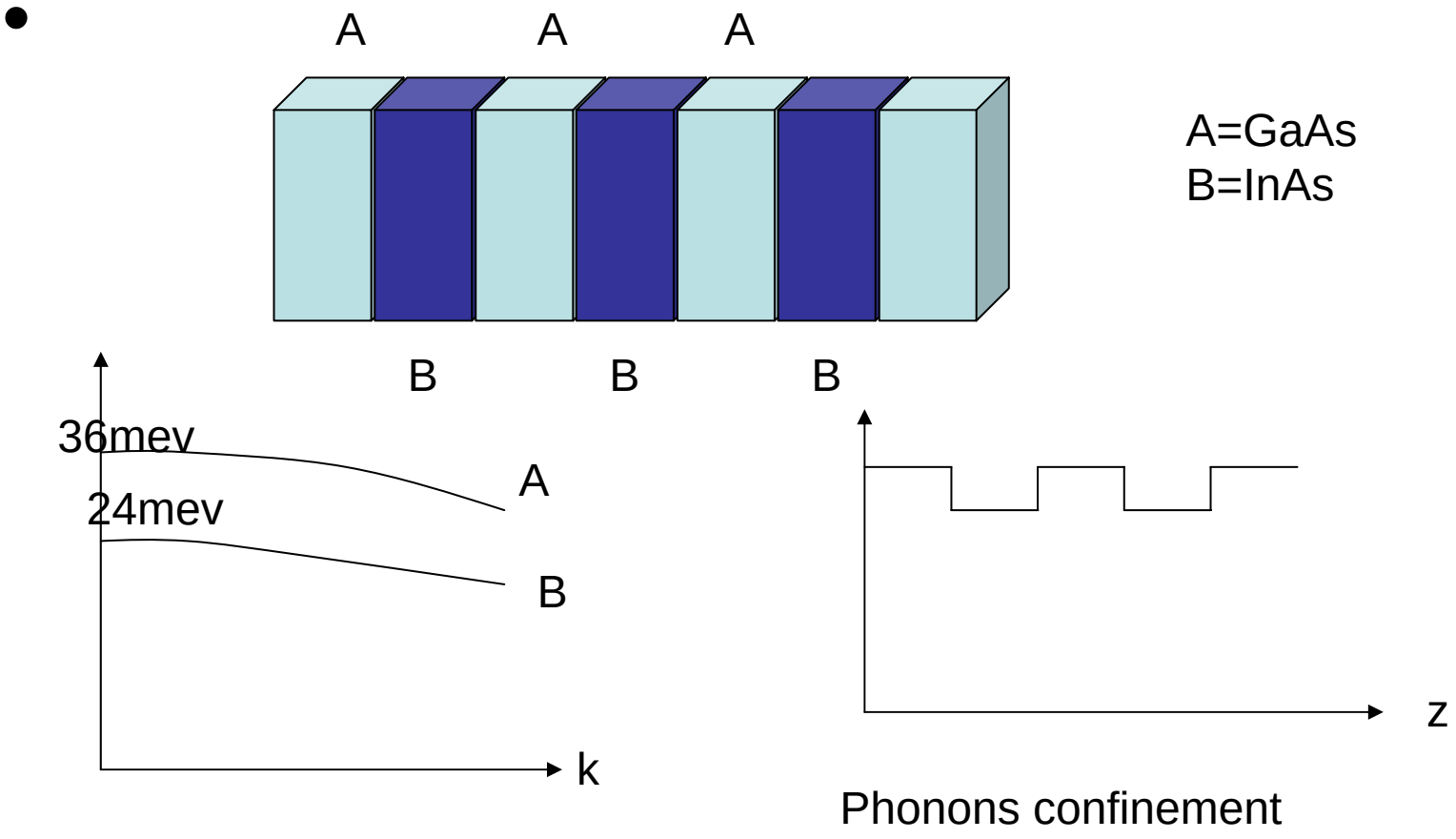
- Wire
(1d)



Dot (0d)

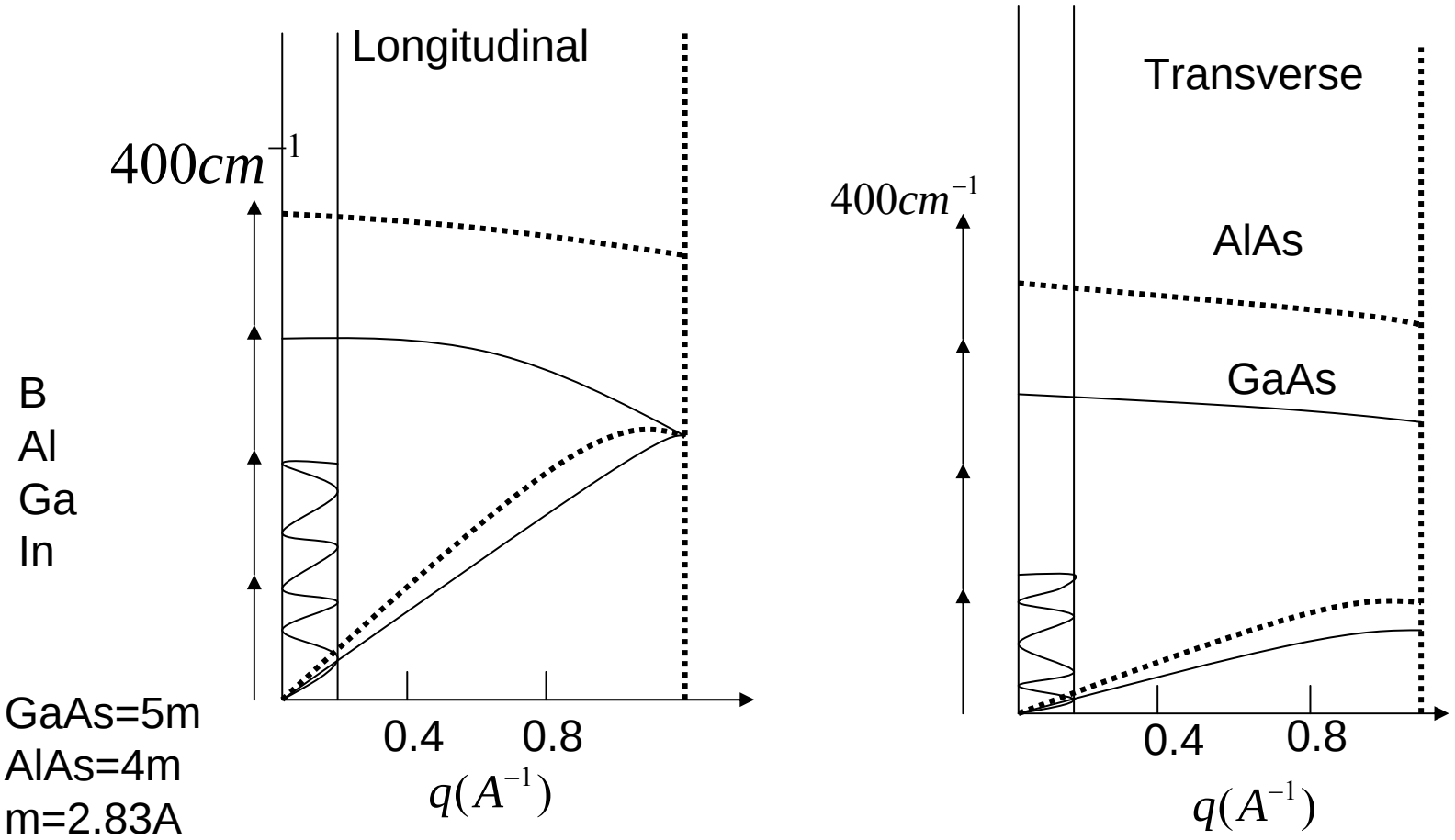


4. Phonons in superlattices

- 

Physical Review B 31,2080 (1985)

- Folded acoustic and quantized optic phonons in GaAs/AlAs



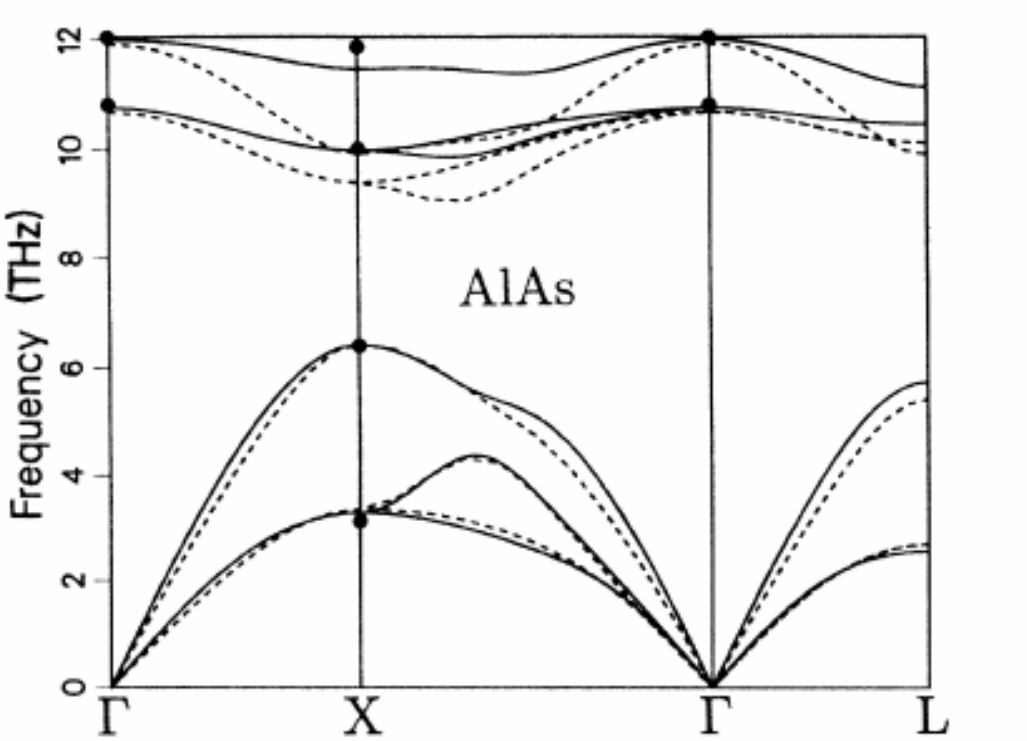


FIG. 1. The dispersion curves of bulk AlAs calculated by using 11-parameter rigid-ion model. The solid curves are the results of parameters fitted to the existing experimental data, and the dashed curves are the results of parameters fitted to the theoretical calculation of Yip and Chang (Ref. 13).

S.-F. Ren, H. Chu, and Y. C. Chang, Phys. Rev. B **37**, 8899 (1988).

Zone-folded Phonons in SL

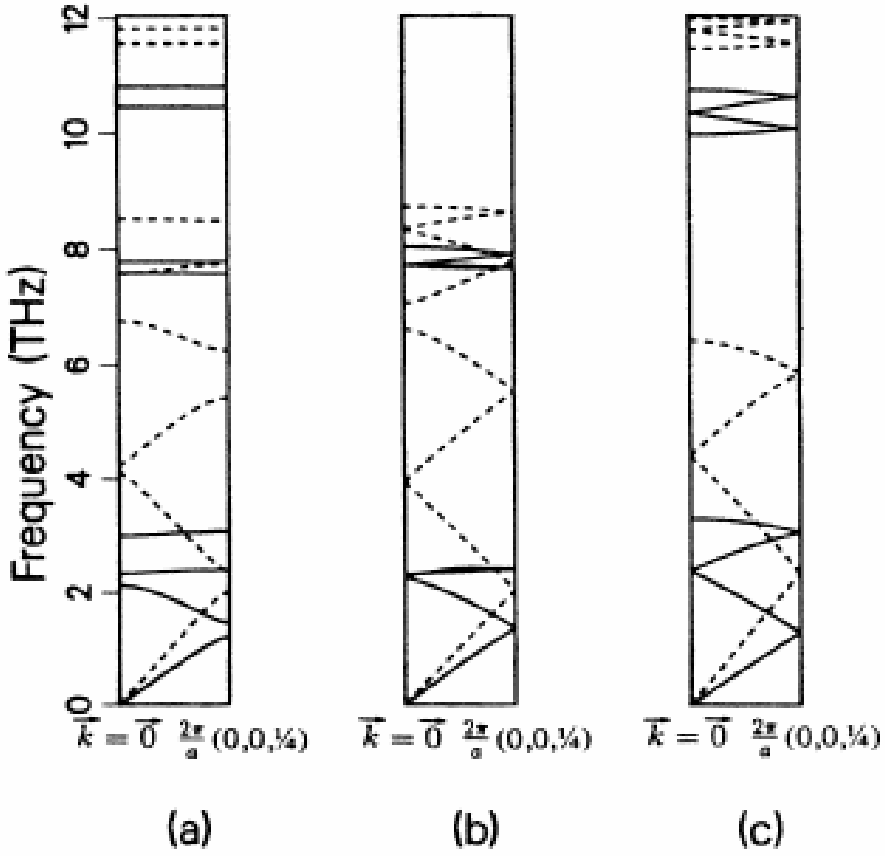


FIG. 2. (a) The dispersion curves of a (2,2) GaAs-AlAs superlattice along [001]; (b) GaAs bulk phonon dispersion curves along [001] folded over the same period as (a); (c) AlAs bulk phonon dispersion curves along [001] folded over the same period as (a). The solid curves are transverse modes (doubly degenerate) and the dashed curves are longitudinal modes.

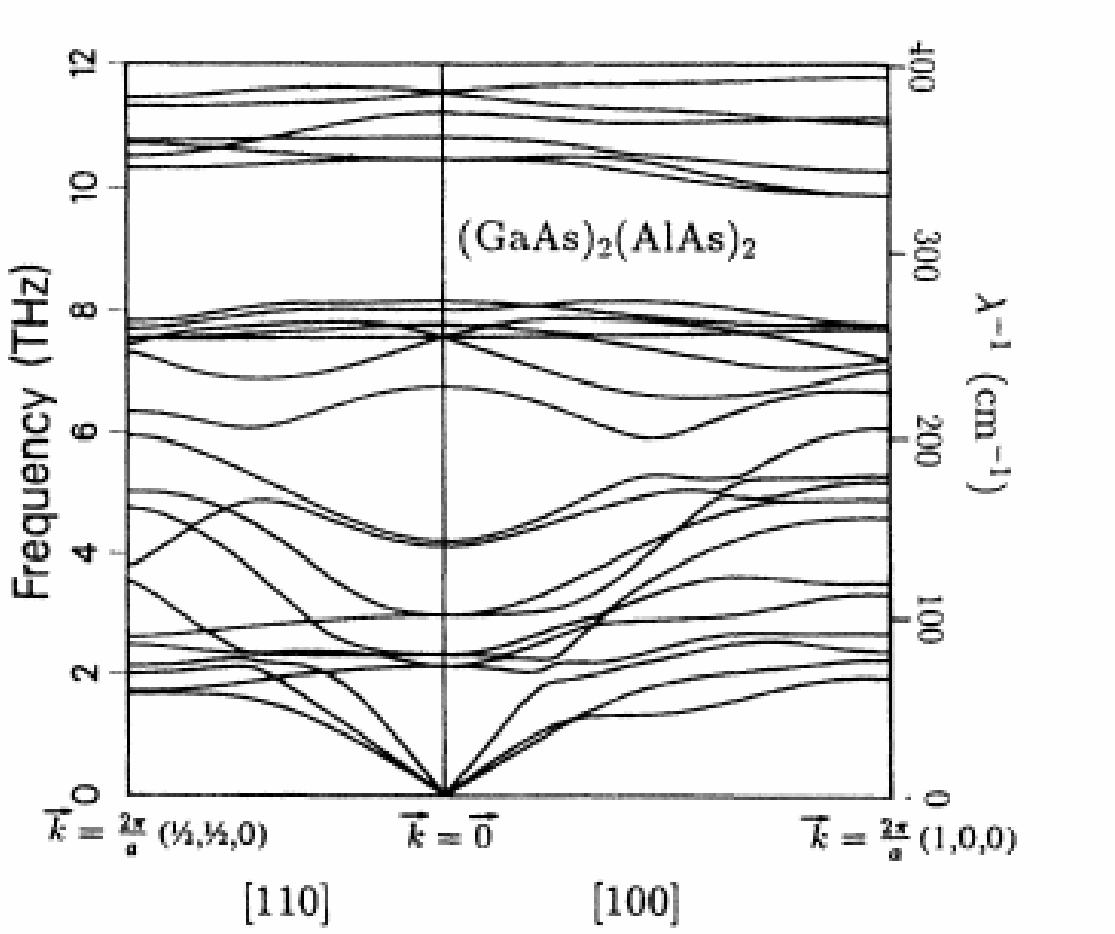


FIG. 3. Dispersion curves of (2,2) GaAs-AlAs superlattice along [110] and [100].

Angular dispersion at k=0

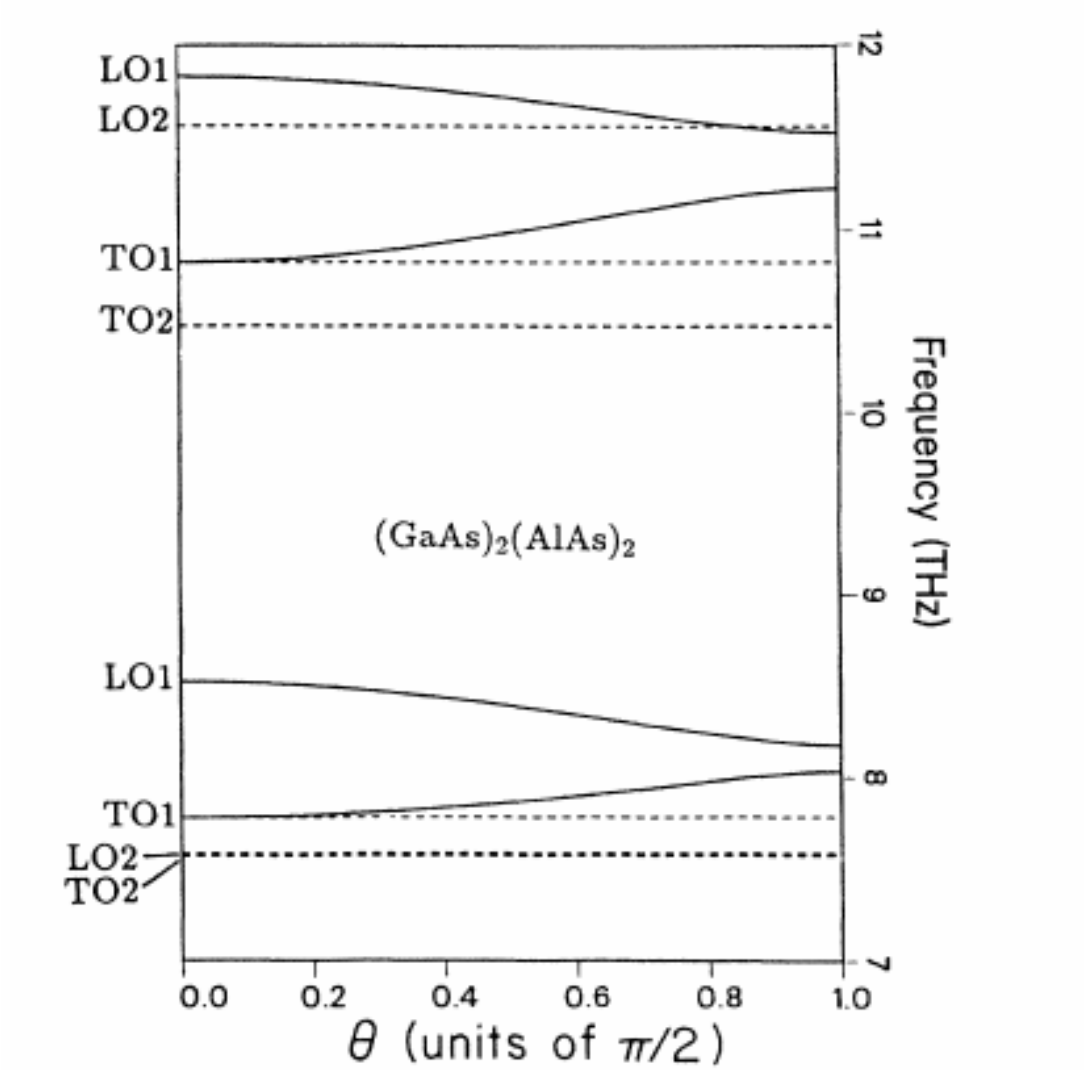


FIG. 4. Frequencies of zone-center ($\mathbf{k}=\mathbf{0}$) optical modes for a (2,2) GaAs-AlAs superlattice as functions of θ.

Angular dispersion at k=0

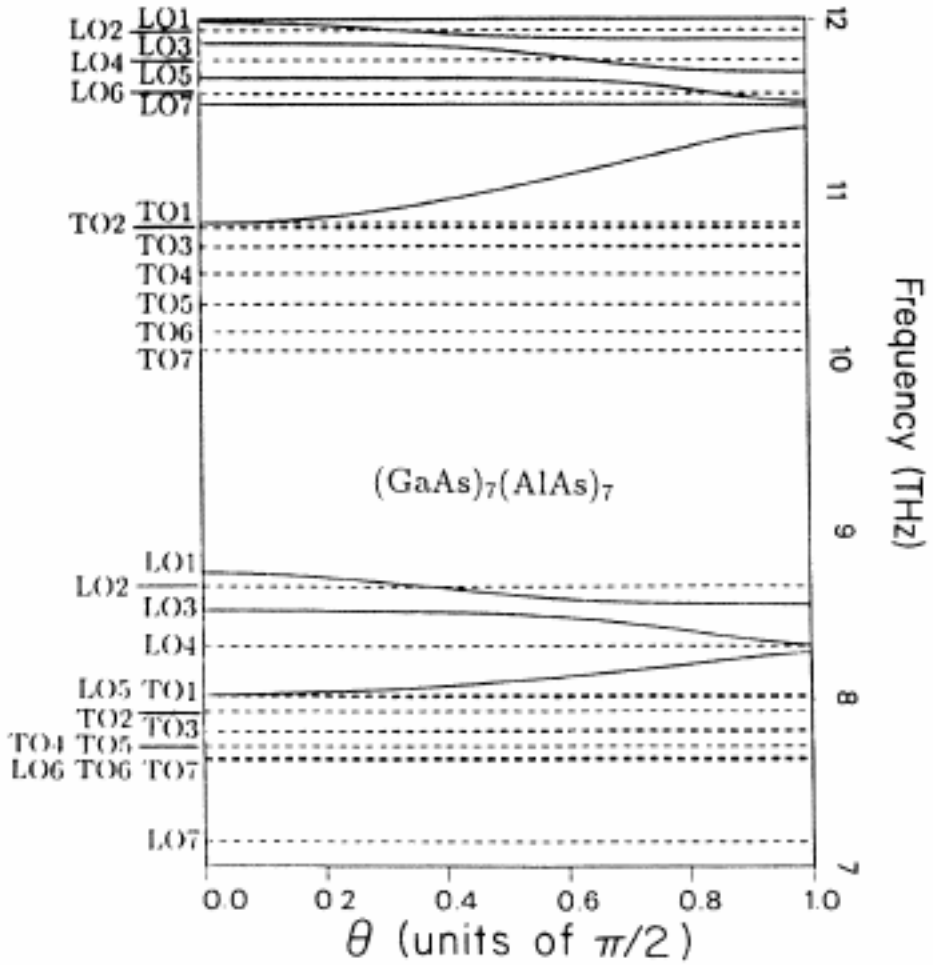


FIG. 6. Angular dependence of the optical phonons at the Brillouin zone center as a function of θ for a (7,7) GaAs-AlAs superlattice.

SL phonon bands

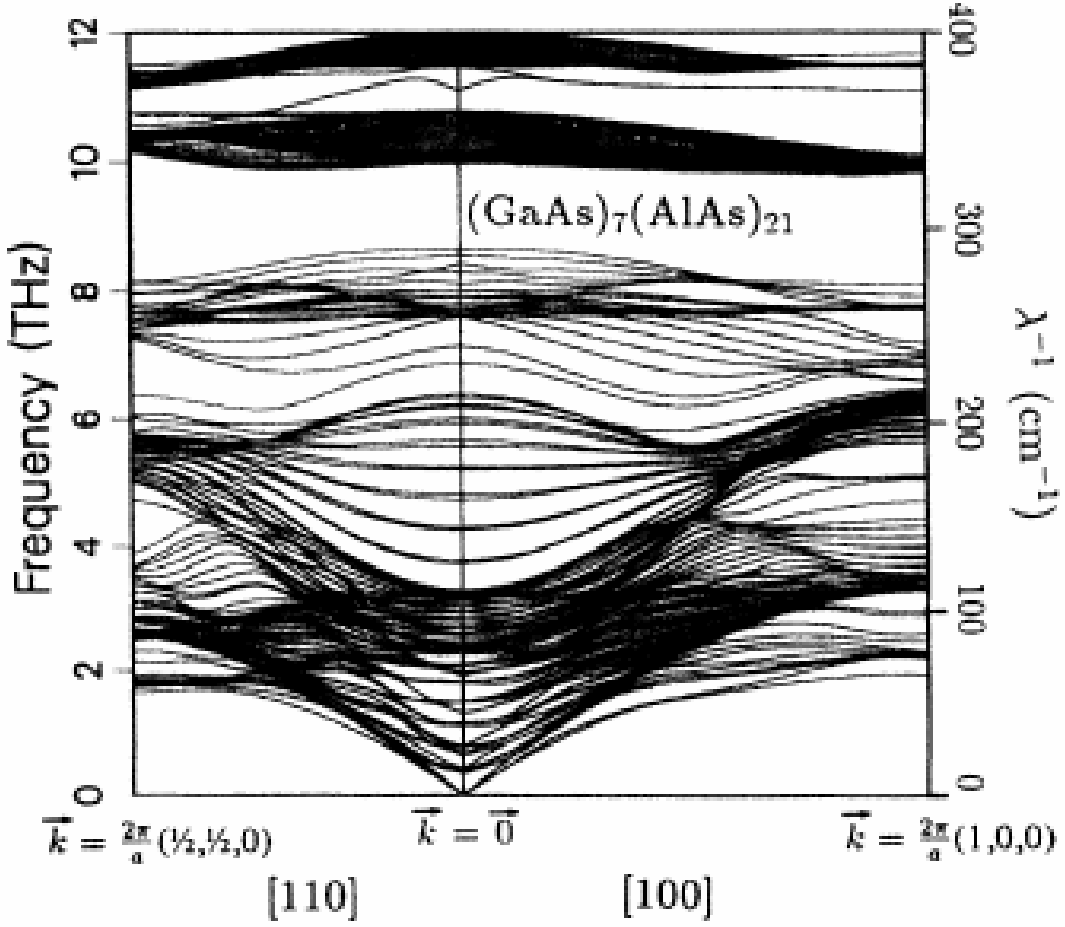


FIG. 12. Dispersion curves of a (7,21) GaAs-AlAs superlattice along [110] and [100].

Projected bulk phonon bands

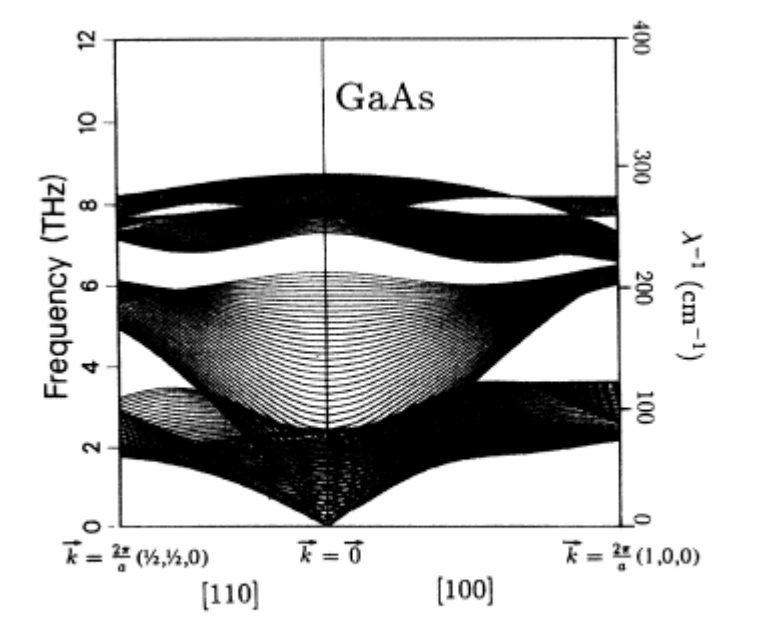


FIG. 13. Projected phonon bands of the bulk of GaAs along [100] and [110].

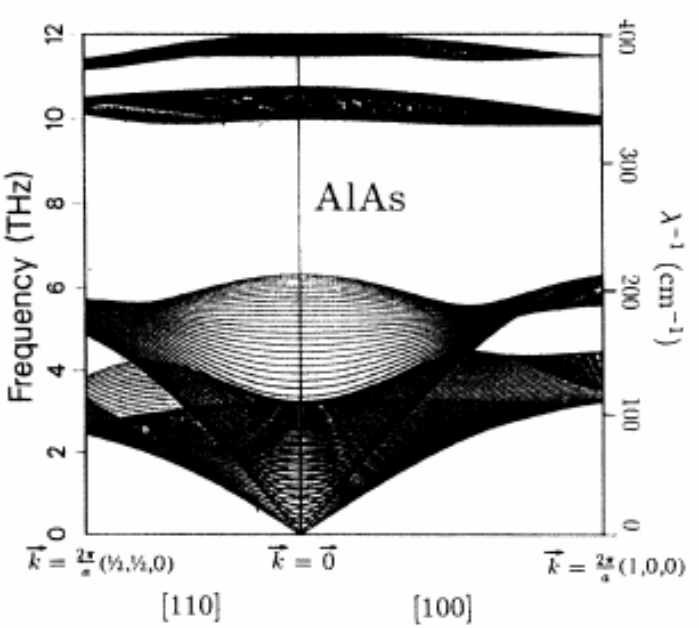


FIG. 14. Projected phonon bands of the bulk of AlAs along [100] and [110].

Extracted interface phonon modes in SL

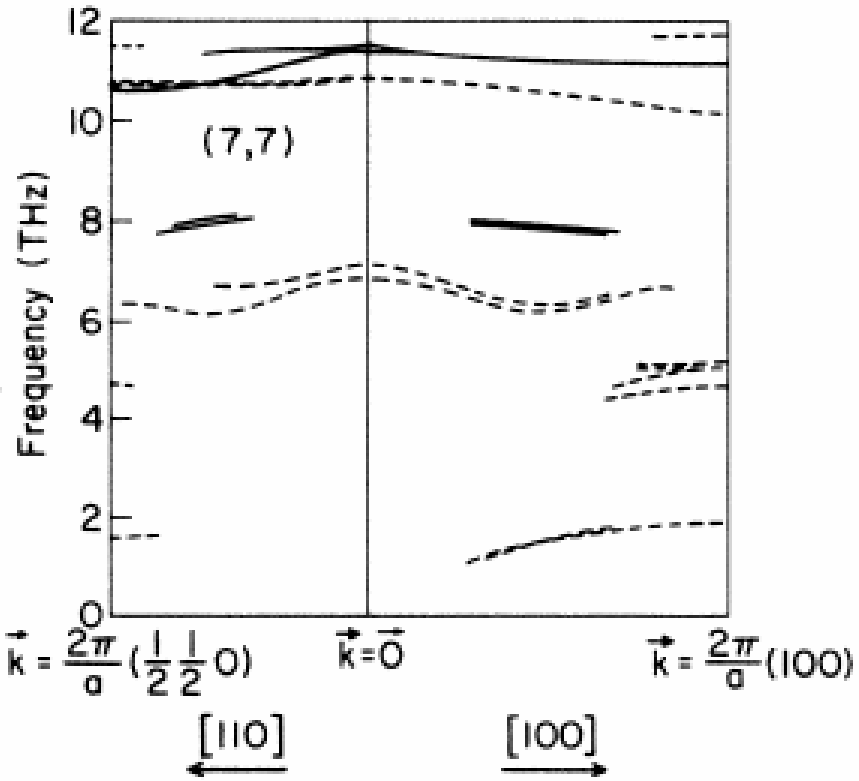
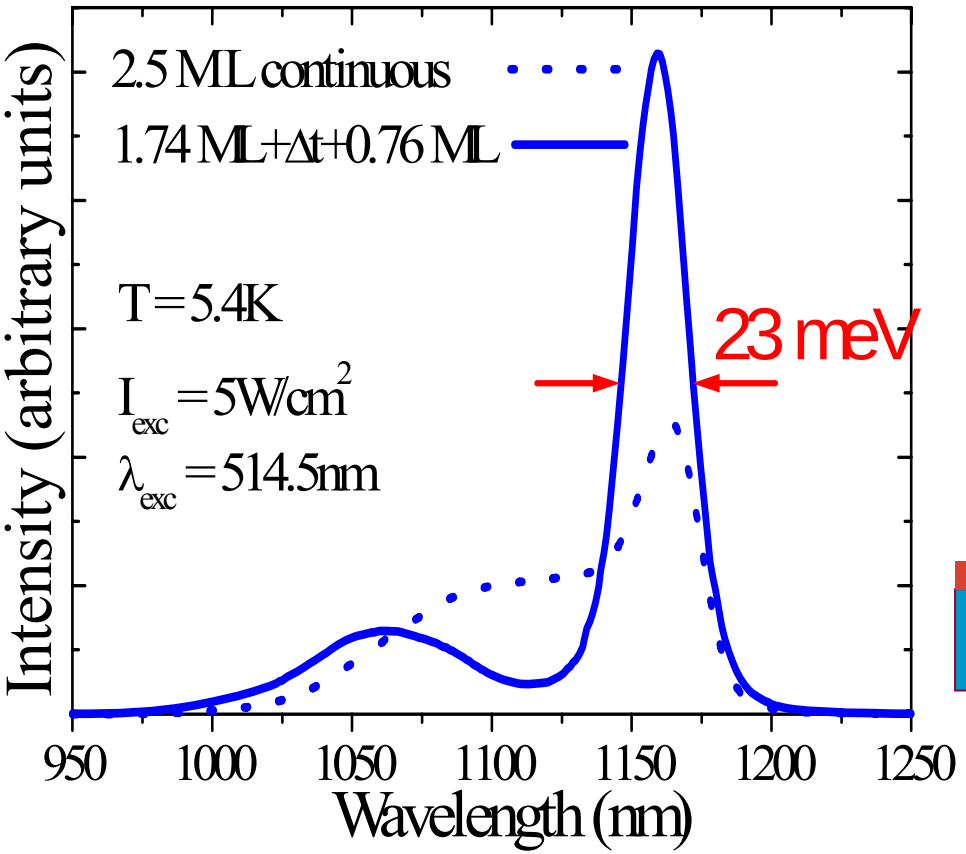
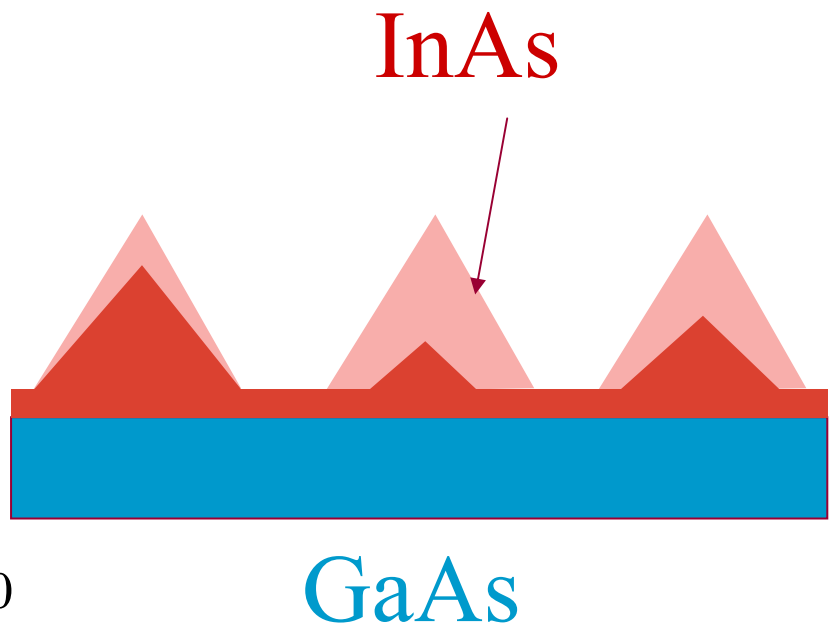


FIG. 15. Dispersion curves of interface modes for the (7,7) GaAs-AlAs superlattice. Solid curves, macroscopic interface modes; dashed curves, microscopic interface modes.

PL of InAs/GaAs self-assembled QDs



Stranski-Krastanov growth



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Phonon bottleneck in QD

- In polar semiconductor
- Quantum dots with discrete states