6.730 Physics for Solid State Applications

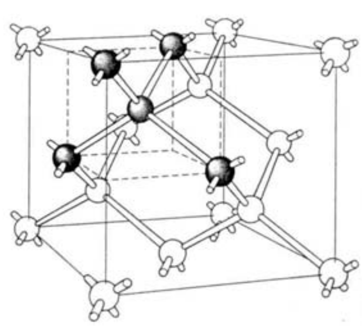
Lecture 10: Lattice Waves in 2D and 3D

Outline

- •Algebra for Bond Stretching in 3-D
- • Example: 2-D Lattice Waves with Bond Stretching
- • Algebra for Bond Bending in 3-D
- • Example: 1-D and 2-D Lattice Waves with Bond Stretching and Bending
- •3-D Examples

February 25, 2004

Lattice Waves in 3-D Crystals



Displacements of basis atoms along three directions...

$$u_{1x}[\mathbf{R_n}] \qquad u_{2x}[\mathbf{R_n}]$$
$$u_{1y}[\mathbf{R_n}] \qquad u_{2y}[\mathbf{R_n}]$$
$$u_{1z}[\mathbf{R_n}] \qquad u_{2z}[\mathbf{R_n}]$$

Lattice Waves in 3-D Crystals

Second order Taylor series expansion for total potential energy:

$$V(\{u[\mathbf{R_s},\mathbf{t}]\}) = \mathbf{V_o} + \frac{1}{2}\sum_{\mathbf{i}}\sum_{\mathbf{j}}\sum_{\mathbf{R_p}}\sum_{\mathbf{R_m}} \mathbf{u_i}[\mathbf{R_p},\mathbf{t}]\,\widetilde{\mathbf{D}}_{\mathbf{i,j}}(\mathbf{R_p},\mathbf{R_m})\,\mathbf{u_j}[\mathbf{R_m},\mathbf{t}]$$

Harmonic Matrix:

$$\widetilde{\mathbf{D}}_{i,j}(\mathbf{R_p},\mathbf{R_m}) = \left(\frac{\partial^2 \mathbf{V}}{\partial \mathbf{u_i}[\mathbf{R_p},\mathbf{t}]\,\partial \mathbf{u_j}[\mathbf{R_m},\mathbf{t}]}\right)_{\text{eq}}$$

Equation of motion for lattice atoms assuming ‘plane wave’ solutions:

$$\left(\mathbf{M}^{-1}\mathbf{D}(\mathbf{k})\right)\vec{\epsilon} = \omega^2\vec{\epsilon}$$

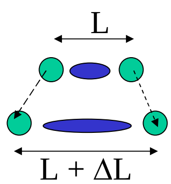
Dynamical Matrix:

$$\mathbf{D_{i,j}}(\mathbf{k}) = \sum_{\mathbf{R_p}}\left(\frac{\partial^2 \mathbf{V}}{\partial \mathbf{u_i}[\mathbf{R_s}+\mathbf{R_p},\mathbf{t}]\,\partial \mathbf{u_j}[\mathbf{R_s},\mathbf{t}]}\right)_{\text{eq}} \mathbf{e}^{-\mathbf{ik}\cdot\mathbf{R_p}}$$

Lattice Waves in 3-D Crystals

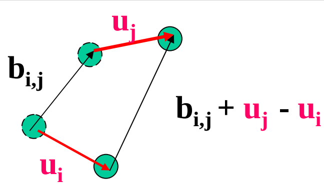
$$\left(\mathbf{M}^{-1}\mathbf{D}(\mathbf{k})\right)\vec{\epsilon} = \omega^2\vec{\epsilon}$$

$$\epsilon[\mathbf{R_n}] = \begin{pmatrix} \epsilon_{1x}[\mathbf{R_n}] \\ \epsilon_{2x}[\mathbf{R_n}] \\ \vdots \\ \epsilon_{1y}[\mathbf{R_n}] \\ \epsilon_{2y}[\mathbf{R_n}] \\ \vdots \\ \epsilon_{1z}[\mathbf{R_n}] \\ \epsilon_{2z}[\mathbf{R_n}] \\ \vdots \end{pmatrix} \quad \mathbf{M} = \begin{pmatrix} M_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & M_2 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & M_1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & M_2 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots\vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & M_1 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & M_2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



Bond Stretching

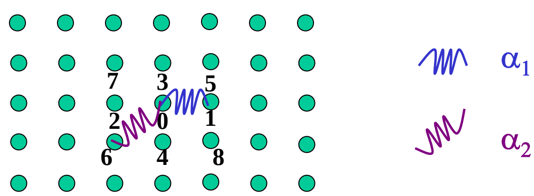
$$E_s = \frac{1}{2}\alpha_s\,(\Delta L)^2$$



$$\Delta L = \left|\mathbf{b} + \mathbf{u_j} - \mathbf{u_i}\right| - |\mathbf{b}| \quad \Longrightarrow \quad \Delta L \approx \hat{\mathbf{b}}_{i,j}\cdot\left(\mathbf{u_j} - \mathbf{u_i}\right)$$

$$E_s = \frac{1}{2}\alpha_s\left(\hat{\mathbf{b}}_{i,j}\cdot\left(\mathbf{u_j} - \mathbf{u_i}\right)\right)^2$$

Example: 2-D Lattice with Bond Stretching



$$V = \cdots + \frac{\alpha_1}{2}\left|\hat{\mathbf{a}}_1\cdot(\mathbf{u}[\mathbf{R}+\mathbf{a}_1]-\mathbf{u}[\mathbf{R}])\right|^2 + \frac{\alpha_1}{2}\left|\hat{\mathbf{a}}_1\cdot(\mathbf{u}[\mathbf{R}-\mathbf{a}_1]-\mathbf{u}[\mathbf{R}])\right|^2$$

$$+\frac{\alpha_1}{2}\left|\hat{\mathbf{a}}_2\cdot(\mathbf{u}[\mathbf{R}+\mathbf{a}_2]-\mathbf{u}[\mathbf{R}])\right|^2 + \frac{\alpha_1}{2}\left|\hat{\mathbf{a}}_2\cdot(\mathbf{u}[\mathbf{R}-\mathbf{a}_2]-\mathbf{u}[\mathbf{R}])\right|^2$$

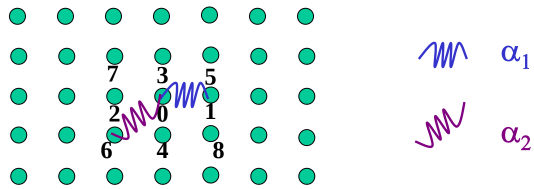
$$+\frac{\alpha_2}{2}\left|\frac{\hat{\mathbf{a}}_1+\hat{\mathbf{a}}_2}{\sqrt{2}}\cdot(\mathbf{u}[\mathbf{R}+\mathbf{a}_1+\mathbf{a}_2]-\mathbf{u}[\mathbf{R}])\right|^2$$

$$+\frac{\alpha_2}{2}\left|\frac{-\hat{\mathbf{a}}_1+\hat{\mathbf{a}}_2}{\sqrt{2}}\cdot(\mathbf{u}[\mathbf{R}-\mathbf{a}_1+\mathbf{a}_2]-\mathbf{u}[\mathbf{R}])\right|^2$$

$$+\frac{\alpha_2}{2}\left|\frac{\hat{\mathbf{a}}_1-\hat{\mathbf{a}}_2}{\sqrt{2}}\cdot(\mathbf{u}[\mathbf{R}+\mathbf{a}_1-\mathbf{a}_2]-\mathbf{u}[\mathbf{R}])\right|^2 + \ldots$$

Example: 2-D Lattice with Bond Stretching

Elements of the Dynamical Matrix



$$\mathrm{D_{xx}(k)} = \alpha_1\left(1-\mathrm{e}^{-\mathrm{ik}\cdot\mathrm{a}_1}\right)+\alpha_1\left(1-\mathrm{e}^{\mathrm{ik}\cdot\mathrm{a}_1}\right)+0+0$$

$$+\frac{\alpha_2}{2}\left(1-e^{-i\mathbf{k}\cdot(\mathbf{a}_1+\mathbf{a}_2)}\right)+\frac{\alpha_2}{2}\left(1-e^{-i\mathbf{k}\cdot(-\mathbf{a}_1-\mathbf{a}_2)}\right)$$

$$+\frac{\alpha_2}{2}\left(1-e^{-i\mathbf{k}\cdot(-\mathbf{a}_1+\mathbf{a}_2)}\right)+\frac{\alpha_2}{2}\left(1-e^{-i\mathbf{k}\cdot(\mathbf{a}_1-\mathbf{a}_2)}\right)$$

Example: 2-D Lattice with Bond Stretching

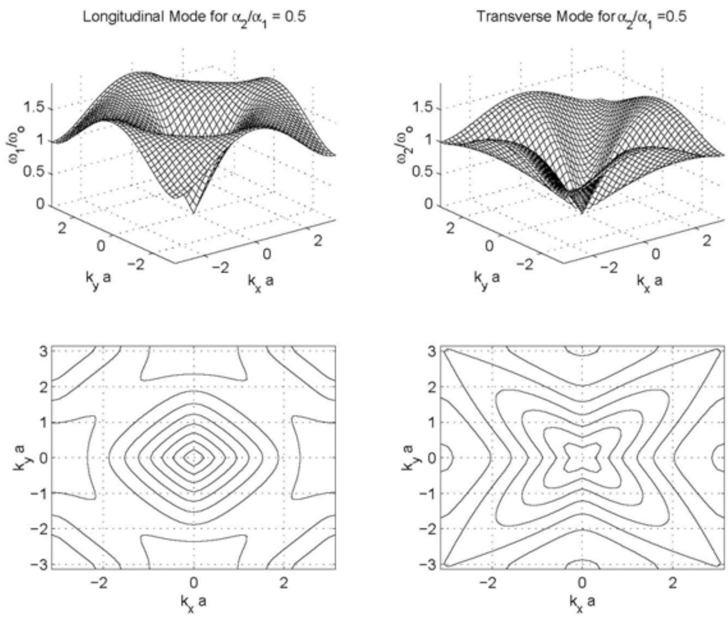
Dynamical Matrix

$$\mathrm{D(k)} = \begin{pmatrix} 2\alpha_1(1-\cos k_x a)+2\alpha_2(1-\cos k_x a\cos k_y a) & 2\alpha_2\sin k_x a\sin k_y a \\ 2\alpha_2\sin k_x a\sin k_y a & 2\alpha_1(1-\cos k_y a)+2\alpha_2(1-\cos k_x a\cos k_y a) \end{pmatrix}$$

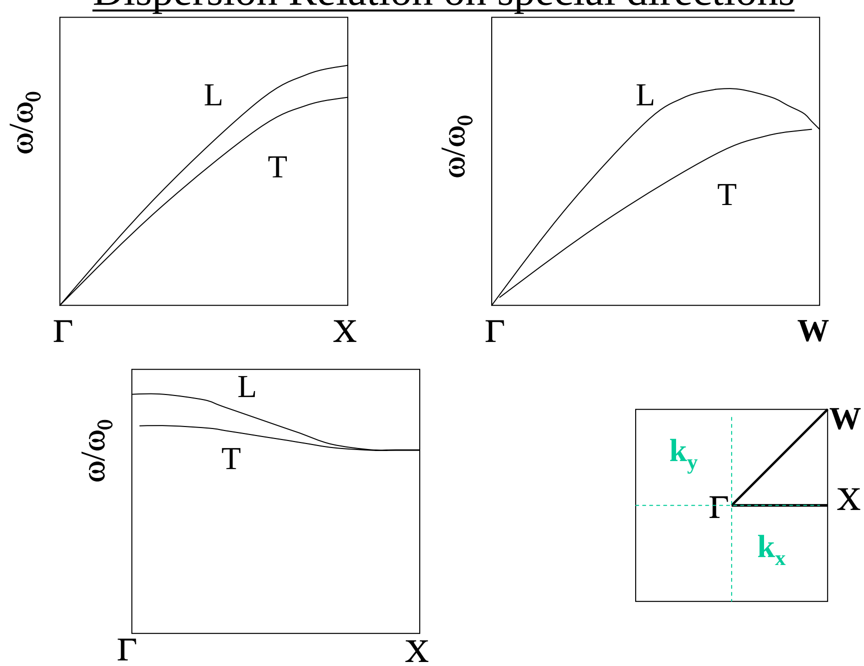
$$\mathbf{M} = \mathrm{M}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\frac{1}{M}\mathbf{D(k)}\tilde{\epsilon} = \omega^2\tilde{\epsilon}$$

2d Dispersion Relation



Dispersion Relation on special directions



Example: 2-D Lattice with Bond Stretching

Dispersion Relation

$$\mathbf{D}(k_x,0) = \begin{pmatrix} 2(\alpha_1+\alpha_2)(1-\cos k_x a) & 0 \\ 0 & 2\alpha_2(1-\cos k_x a) \end{pmatrix}$$

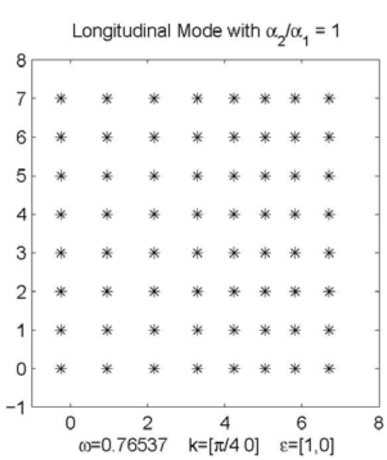
$$\omega_1(k_x,0) = \sqrt{\frac{4(\alpha_1+\alpha_2)}{M}}\sin\frac{k_x a}{2} \qquad \vec{\epsilon}_1(k_x,0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

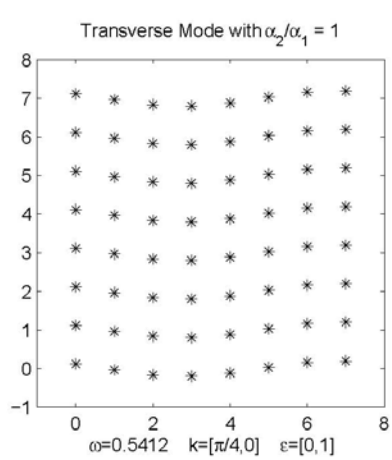
$$\omega_2(k_x,0) = \sqrt{\frac{4\alpha_2}{M}}\sin\frac{k_x a}{2} \qquad \vec{\epsilon}_2(k_x,0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\tilde{u}_i[\mathbf{R_n},\mathbf{t}] = \mathbf{e}^{\mathbf{i}(\mathbf{k}\cdot\mathbf{R_n}-\omega_\mathbf{i}(\mathbf{k})\mathbf{t})}\,\tilde{\epsilon}_\mathbf{i}(\mathbf{k})$$

2D Modes

$$\mathbf{D}(\mathbf{k}) = \begin{pmatrix} 4\alpha_{sA}\sin^2\frac{\mathbf{k}\cdot\mathbf{a_1}}{2} + 4\alpha_{\phi B}\sin^2\frac{\mathbf{k}\cdot\mathbf{a_2}}{2} & 0 \\ 0 & 4\alpha_{sB}\sin^2\frac{\mathbf{k}\cdot\mathbf{a_2}}{2} + 4\alpha_{\phi A}\sin^2\frac{\mathbf{k}\cdot\mathbf{a_1}}{2} \end{pmatrix}$$





Example: 2-D Lattice with Bond Stretching

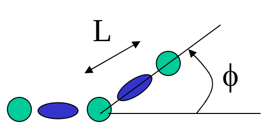
Relating Microscopic and Macroscopic Models

$$\omega_1(k_x,0) \approx \underbrace{\sqrt{\frac{(\alpha_1+\alpha_2)a^2}{M}}}_{c_L} k_x \qquad \text{and} \qquad \omega_2(k_x,0) \approx \underbrace{\sqrt{\frac{\alpha_2 a^2}{M}}}_{c_T} k_x$$

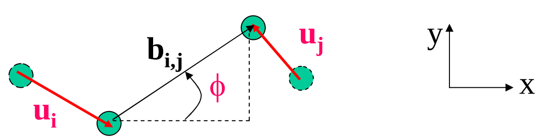
$$c_L = \sqrt{(\lambda+2\mu)/\rho} \qquad \text{and} \qquad c_T = \sqrt{\mu/\rho}$$

$$\mu = \alpha_2 \qquad \text{and} \qquad \lambda = \alpha_1 - \alpha_2$$

Bond Bending



$$E_\phi = \frac{1}{2}\alpha_\phi L^2 (\Delta\phi)^2$$

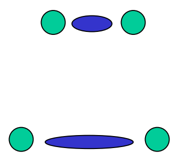


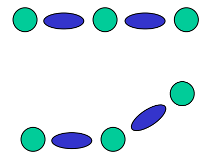
$$\tan(\Delta\phi) = \frac{\mathrm{u_{jy}} - \mathrm{u_{iy}}}{L + \Delta L} \quad \Rightarrow \quad (\Delta\phi) = \frac{\mathrm{u_{jy}} - \mathrm{u_{iy}}}{L}$$

$$\mathbf{u_{iy}} = \mathbf{u_i} - \hat{\mathbf{b}}_{\mathbf{i,j}}\left(\hat{\mathbf{b}}_{\mathbf{i,j}} \cdot \mathbf{u_i}\right) \qquad L^2(\Delta\phi)^2 = \left|\mathbf{u_{iy}} - \mathbf{u_{jy}}\right|^2$$

$$E_\phi = \frac{1}{2}\alpha_\phi\left(\left|\mathbf{u_i} - \mathbf{u_j}\right|^2 - \left[\hat{\mathbf{b}}_{i,j} \cdot \left(\mathbf{u_i} - \mathbf{u_j}\right)\right]^2\right)$$

Bond Stretching and Bending



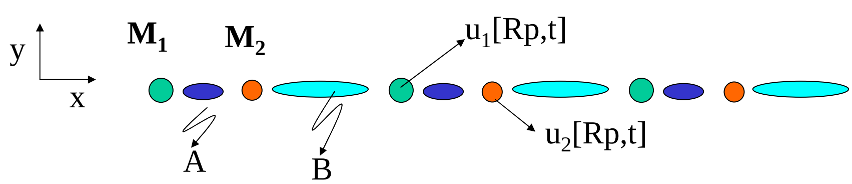


$$E_s = \frac{1}{2}\alpha_s\,(\Delta L)^2 \qquad E_\phi = \frac{1}{2}\alpha_\phi L^2(\Delta\phi)^2$$

$$E_s = \frac{1}{2}\alpha_s\left(\hat{\mathbf{b}}_{i,j}\cdot\left(\mathbf{u_j}-\mathbf{u_i}\right)\right)^2 \qquad E_\phi = \frac{1}{2}\alpha_\phi\left(\left|\mathbf{u_i}-\mathbf{u_j}\right|^2-\left[\hat{\mathbf{b}}_{i,j}\cdot\left(\mathbf{u_i}-\mathbf{u_j}\right)\right]^2\right)$$

Example: 1-D Diatomic Lattice with Bond Stretching and Bending

Potential Energy



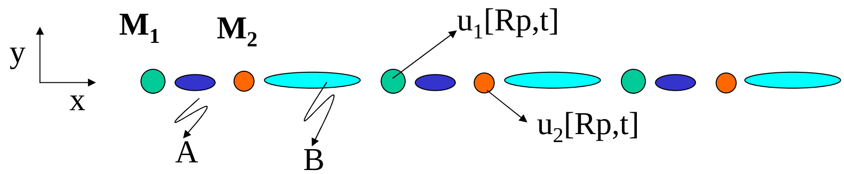
$$E_s = \frac{1}{2}\alpha_s\,(\Delta L)^2 \qquad E_\phi = \frac{1}{2}\alpha_\phi L^2(\Delta\phi)^2$$

$$E_s = \frac{1}{2}\alpha_s\left(\hat{\mathbf{b}}_{i,j}\cdot\left(\mathbf{u_j}-\mathbf{u_i}\right)\right)^2 \qquad E_\phi = \frac{1}{2}\alpha_\phi\left(\left|\mathbf{u_i}-\mathbf{u_j}\right|^2-\left[\hat{\mathbf{b}}_{i,j}\cdot\left(\mathbf{u_i}-\mathbf{u_j}\right)\right]^2\right)$$

$$E_s = \frac{1}{2}\alpha_{sA}\left(\mathbf{u_{1x}}[\mathrm{R}]-\mathbf{u_{2x}}[\mathrm{R}]\right)^2 \qquad E_\phi = \frac{1}{2}\alpha_\phi\left|\mathbf{u_{1y}}-\mathbf{u_{2y}}\right|^2$$

Example: '1-D' Diatomic Lattice with Bond Stretching and Bending

Potential Energy

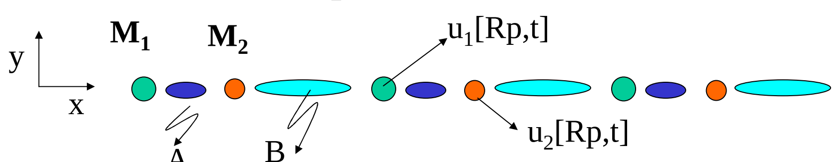


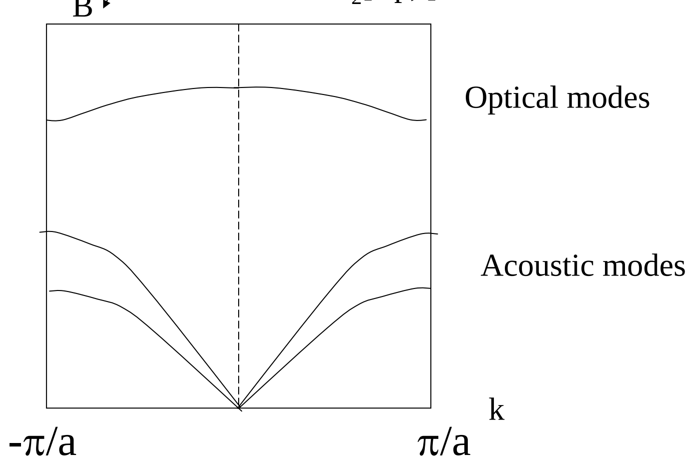
$$V = \ldots \frac{1}{2}\alpha_{sA}\left(\mathbf{u_{1x}}[\mathbf{R}] - \mathbf{u_{2x}}[\mathbf{R}]\right)^2 + \frac{1}{2}\alpha_{\phi A}\left(\mathbf{u_{1y}}[\mathbf{R}] - \mathbf{u_{2y}}[\mathbf{R}]\right)^2$$

$$+\frac{1}{2}\alpha_{sB}\left(\mathbf{u_{1x}}[\mathbf{R}] - \mathbf{u_{2x}}[\mathbf{R}-\mathbf{a}]\right)^2 + \frac{1}{2}\alpha_{\phi B}\left(\mathbf{u_{1y}}[\mathbf{R}] - \mathbf{u_{2y}}[\mathbf{R}-\mathbf{a}]\right)^2 + \ldots$$

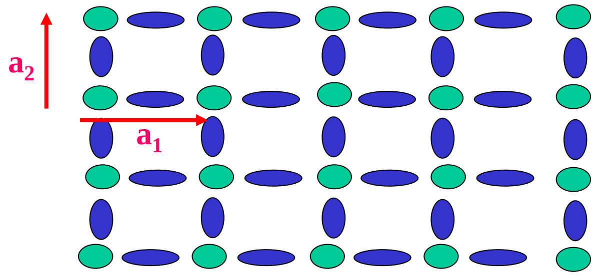
$$\mathbf{D}(\mathbf{k}) = \begin{array}{c} \\ \mathbf{u_{1x}} \\ \mathbf{u_{2x}} \\ \mathbf{u_{1y}} \\ \mathbf{u_{2x}} \end{array} \begin{array}{cccc} \mathbf{u_{1x}} & \mathbf{u_{2x}} & \mathbf{u_{1y}} & \mathbf{u_{2y}} \\ \alpha_{sA}+\alpha_{sB} & -\alpha_{sA}-\alpha_{sB}e^{-ika} & 0 & 0 \\ -\alpha_{sA}-\alpha_{sB}e^{ika} & \alpha_{sA}+\alpha_{sB} & 0 & 0 \\ 0 & 0 & \alpha_{\phi A}+\alpha_{\phi B} & -\alpha_{\phi A}-\alpha_{\phi B}e^{-ika} \\ 0 & 0 & -\alpha_{\phi A}-\alpha_{\phi B}e^{ika} & \alpha_{\phi A}+\alpha_{\phi B} \end{array}$$

1-D DiatomicLattice with Bond Stretching and Bending Dispersion Relation

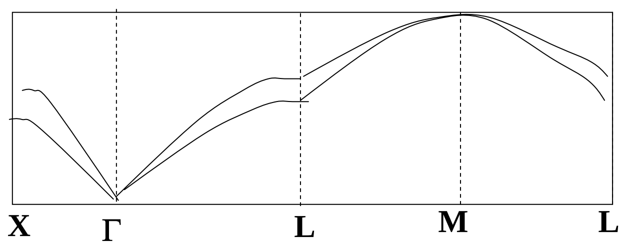


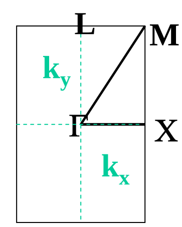


2d rectangular monatomic crystal



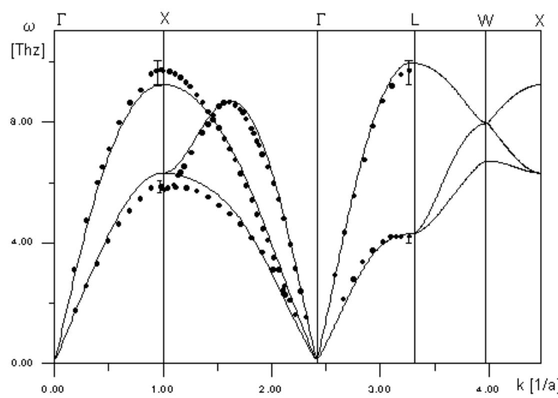
$$D(k) = \begin{pmatrix} 4\alpha_{sA}\sin^2\frac{k\cdot a_1}{2} + 4\alpha_{\phi B}\sin^2\frac{k\cdot a_2}{2} & 0 \\ 0 & 4\alpha_{sB}\sin^2\frac{k\cdot a_2}{2} + 4\alpha_{\phi A}\sin^2\frac{k\cdot a_1}{2} \end{pmatrix}$$





Phonon Dispersion in 3D Cubic Crystal

aluminum



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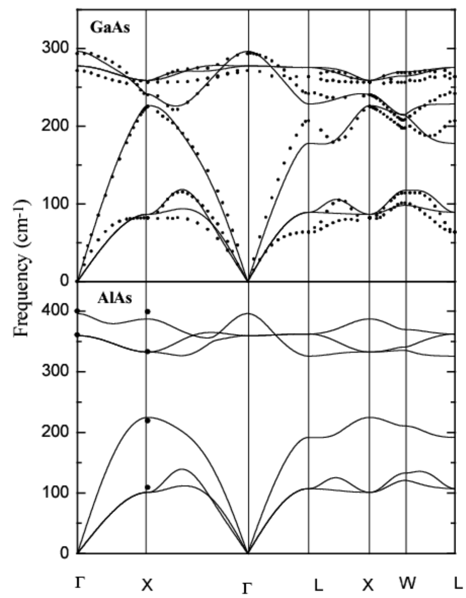
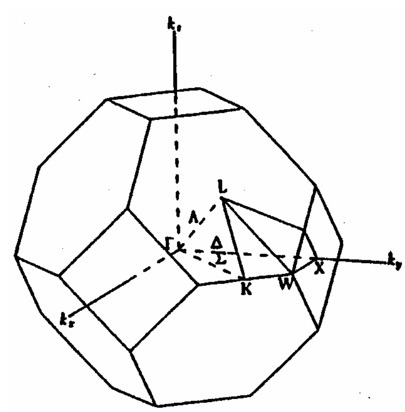
Phonon Dispersion in FCC with 2 Atom Basis





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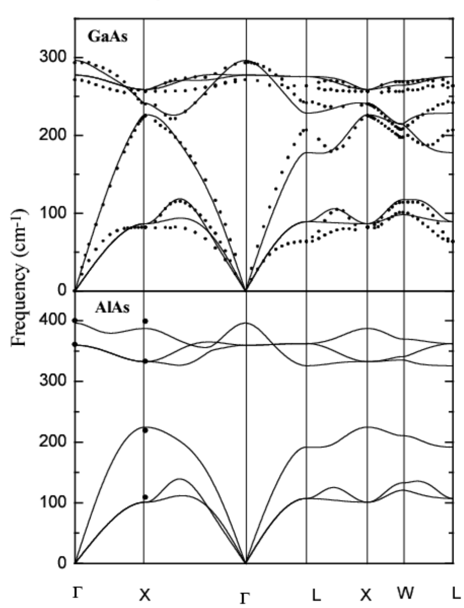
Phonon Dispersion in FCC with 2 Atom Basis



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