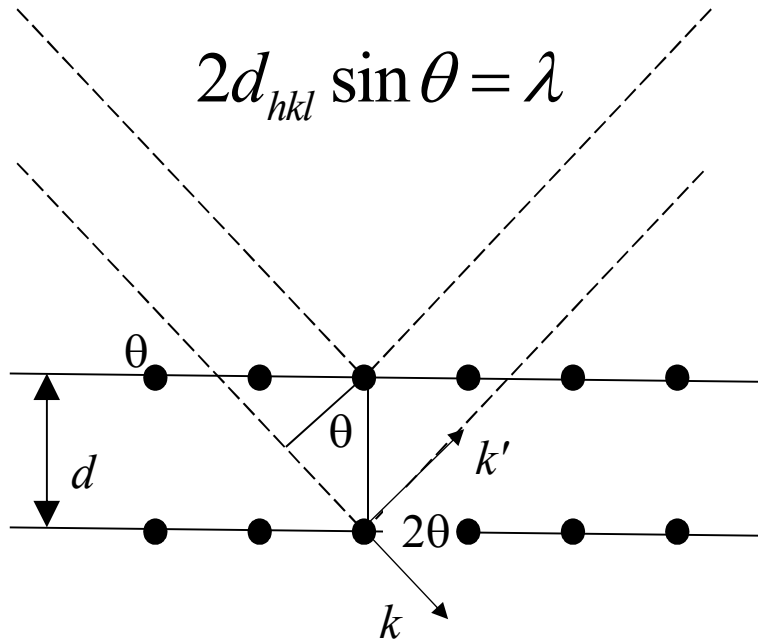


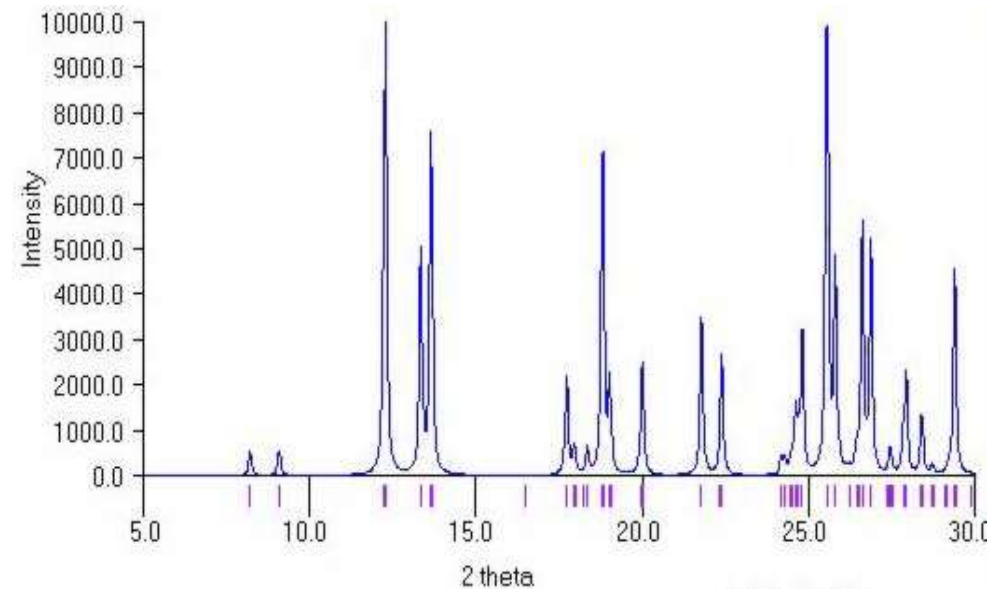
Diffraction Phonons

Powder diffraction

Powder diffraction is performed on a powder of many small crystals. Ideally, every possible crystalline orientation is represented equally in a powdered sample. The relative intensities of the diffraction peaks indicate which crystal structures are present.

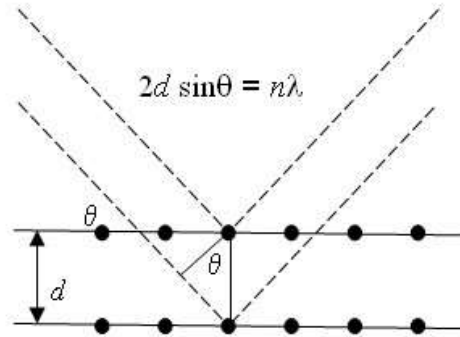


X-rays: Bragg diffraction

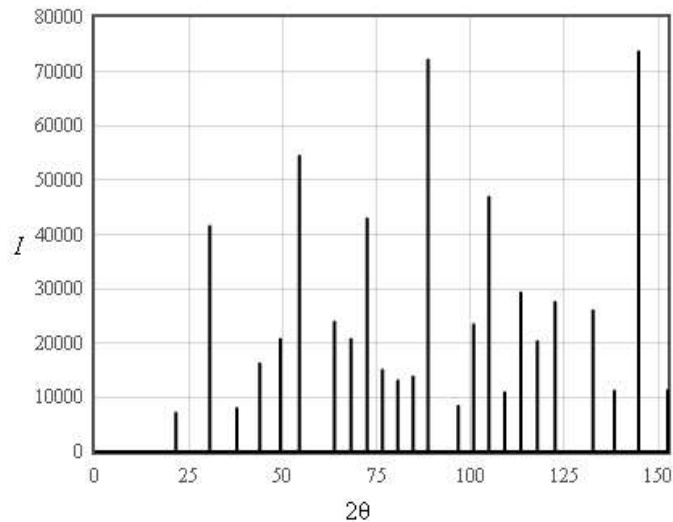


Powder diffraction

For powder diffraction, a crystal is ground into a fine powder so that there are many small crystals with random orientations. X-rays strike the surface of the sample at an angle θ and an x-ray detector is placed at an angle θ to the surface. Only planes parallel to the surface will diffract x-rays to the detector.



Since there are many small crystals with random orientations in the sample, all possible crystal planes that can diffract the x-rays will contribute to the measured signal when θ satisfies the Bragg condition. The form below can calculate the powder diffraction pattern for any crystal with up to five atoms per primitive unit cell. Some buttons are provided that load the form with the data for certain crystals.



Primitive lattice vectors:

$$\vec{a}_1 = 4.12\text{E-}10 \hat{x} + 0 \hat{y} + 0 \hat{z} \text{ [m]}$$

$$\vec{a}_2 = 0 \hat{x} + 4.12\text{E-}10 \hat{y} + 0 \hat{z} \text{ [m]}$$

$$\vec{a}_3 = 0 \hat{x} + 0 \hat{y} + 4.12\text{E-}10 \hat{z} \text{ [m]}$$

Basis:
The positions of the atoms are given in fractional coordinates between -1 and 1.

Cs1+ <input type="button" value="v"/>	0	$\vec{a}_1 +$	0	$\vec{a}_2 +$	0	\vec{a}_3
Cl1- <input type="button" value="v"/>	0.5	$\vec{a}_1 +$	0.5	$\vec{a}_2 +$	0.5	\vec{a}_3
<input type="button" value="v"/>		$\vec{a}_1 +$		$\vec{a}_2 +$		\vec{a}_3
<input type="button" value="v"/>		$\vec{a}_1 +$		$\vec{a}_2 +$		\vec{a}_3
<input type="button" value="v"/>		$\vec{a}_1 +$		$\vec{a}_2 +$		\vec{a}_3

X-ray wavelength λ [\AA] = 1.540598 Cu K α

-

http://rruff.geo.arizona.edu/AMS/all_minerals.php


American Mineralogist Crystal Structure Database

Abellaite	Abelsonite	Abenakiite-(Ce)	Abernathyite	Abhurite
Abswurbachite	Acanthite	Acetamide	Acetylene-hydrate	Achavalite
Actinium	Actinolite	Acuminite	Adachiite	Adamantane
Adamantane-methane-hydrate	Adamite	Adamsite-(Y)	Adelite	Admontite
Adolfpateraite	Adranosite	Adranosite-(Fe)	Aegirine	Aenigmatite
Aerinite	Aerugite	Aeschynite-(La)	Aeschynite-(Y)	Afghanite
Afrite	Afwillite			
Agardite-(Y)	Agrellite			
Ahlfeldite	Ahrensrite			
Ajoite	Akaganeite			
Akhtenskite	Akimotoite			
Aktashite	Alabandite			
Albertiniite	Albite			
Alcaparrosaite	Alflarsenite			
Algodonite	Alinite			
Allanite-(Ce)	Allanite-(La)			
Allantoin	Allargentum			
Allorite	Alluaivite			
Almeidaite	Alnaperboei			
Altaite	Althausite			
Alum-(Na)	Aluminite			
Aluminoceledonite	Aluminocerite			
Aluminotaramite	Aluminum			
Alumotantite	Alunite			
Amarantite	Amarillite			
Americium	Amesite			

American Mineralogist Crystal Structure Database

4 matching records for this search.

Aluminium

 Wyckoff R W G

Crystal Structures 1 (1963) 7-83

Second edition. Interscience Publishers, New York, New York

Cubic closest packed, ccp, structure

_database_code_amcsd 0011137

4.04958 4.04958 4.04958 90 90

atom x y z

Al 0 0 0

[Download AMC data \(View Text File\)](#)

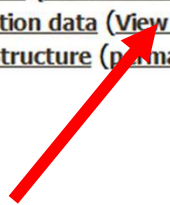
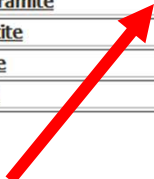
[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

[View JMOl 3-D Structure \(pmlink\)](#)

Aluminium
Wyckoff R W G
Crystal Structures 1 (1963) 7-83
Second edition. Interscience Publishers, New York, New York
Cubic closest packed, ccp, structure
_database_code_amcsd 0011137
CELL PARAMETERS: 4.0496 4.0496 4.0496 90.000 90.000 90.000
SPACE GROUP: Fm3m
X-RAY WAVELENGTH: 1.541838
Cell Volume: 66.409
Density (g/cm3): 2.698
MAX. ABS. INTENSITY / VOLUME**2: 34.61439413
RIR: 4.177
RIR based on corundum from Acta Crystallographica A38 (1982) 733-739
2-THETA INTENSITY D-SPACING H K L Multiplicity
38.50 100.00 2.3380 1 1 1 8
44.76 47.49 2.0248 2 0 0 6
65.16 28.01 1.4317 2 2 0 12
78.30 30.71 1.2210 3 1 1 24
82.52 8.74 1.1690 2 2 2 8

XPOW Copyright 1993 Bob Downs, Ranjini Swaminathan and Kurt Bartelmehs
reference, see Downs et al. (1993) American Mineralogist 78, 1104-1107.





Materials Explorer

Diffraction Patterns i

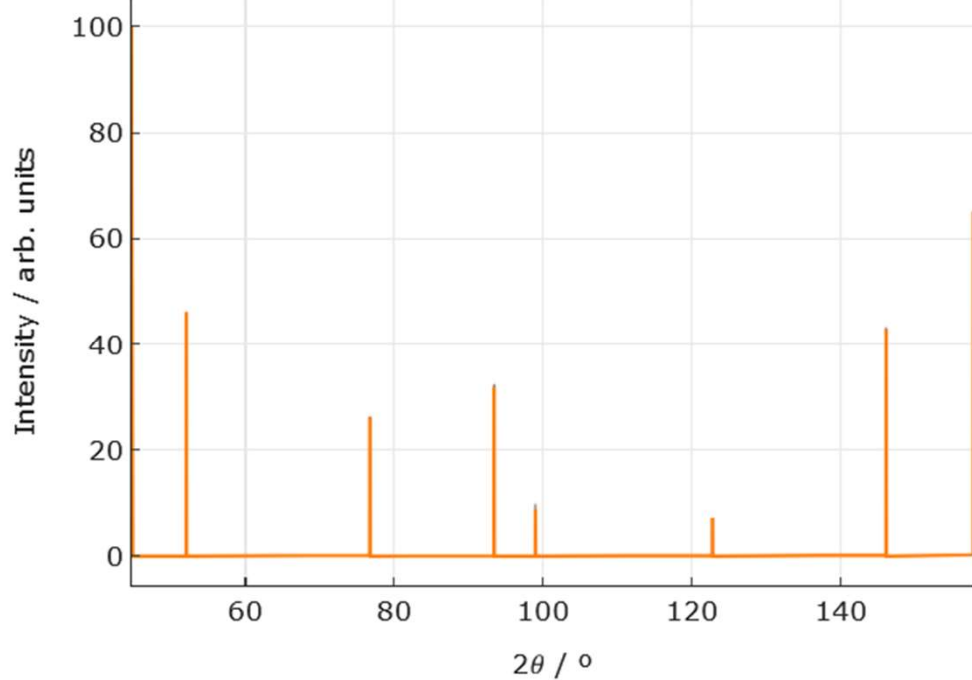
Data Methods API

Mode

X-ray Diffraction (Powder) v

X-ray Diffraction Pattern

Click to enter Plot subtitle



Radiation source

CuKα (1.542 Å) v

Shape Factor

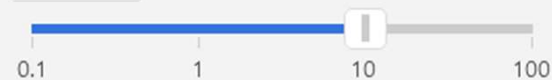
0.94 v

Peak Profile

Gaussian v

Scherrer crystallite size / nm

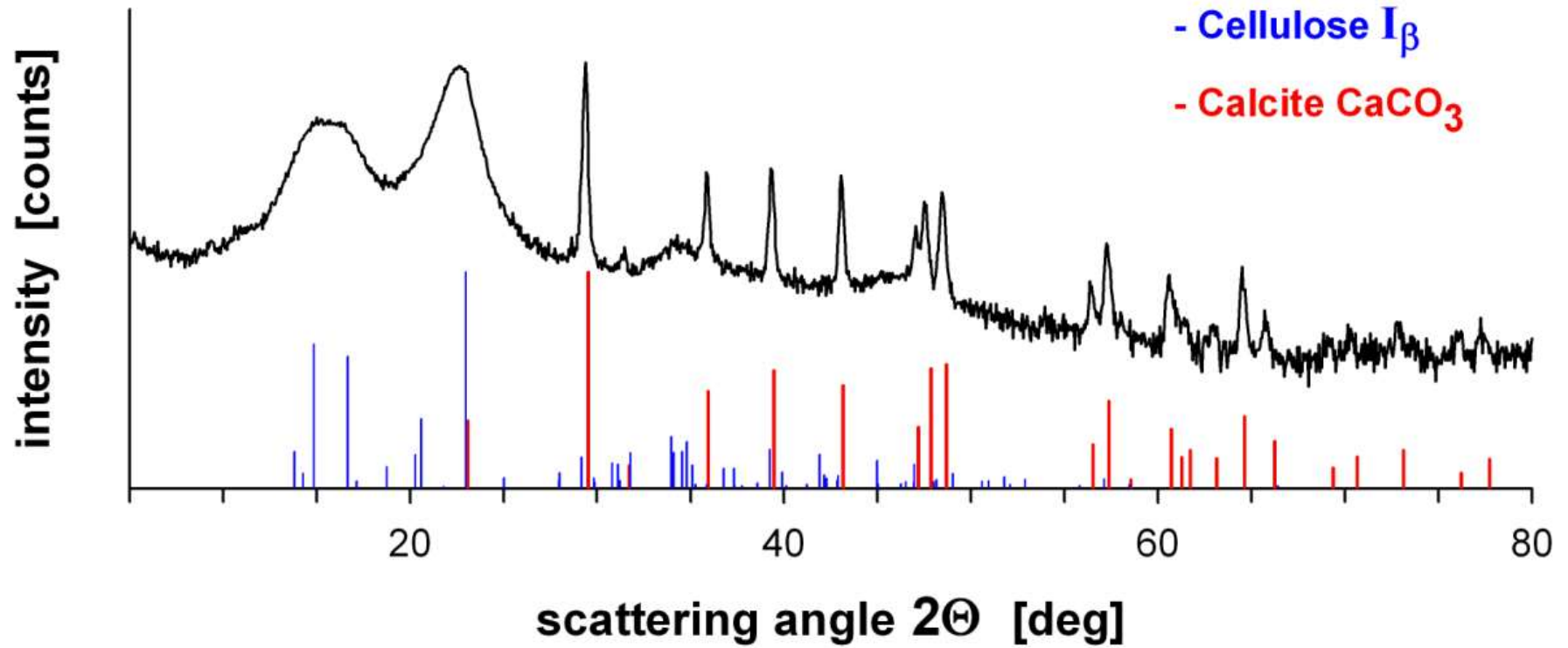
10 v



copy paper

- Cellulose I_β

- Calcite CaCO₃



Powder diffraction

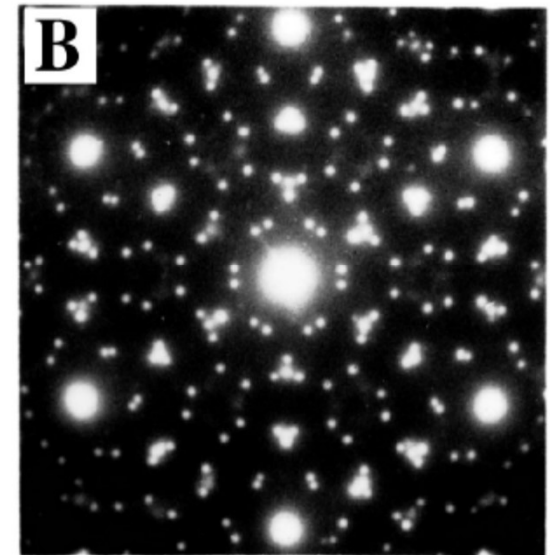
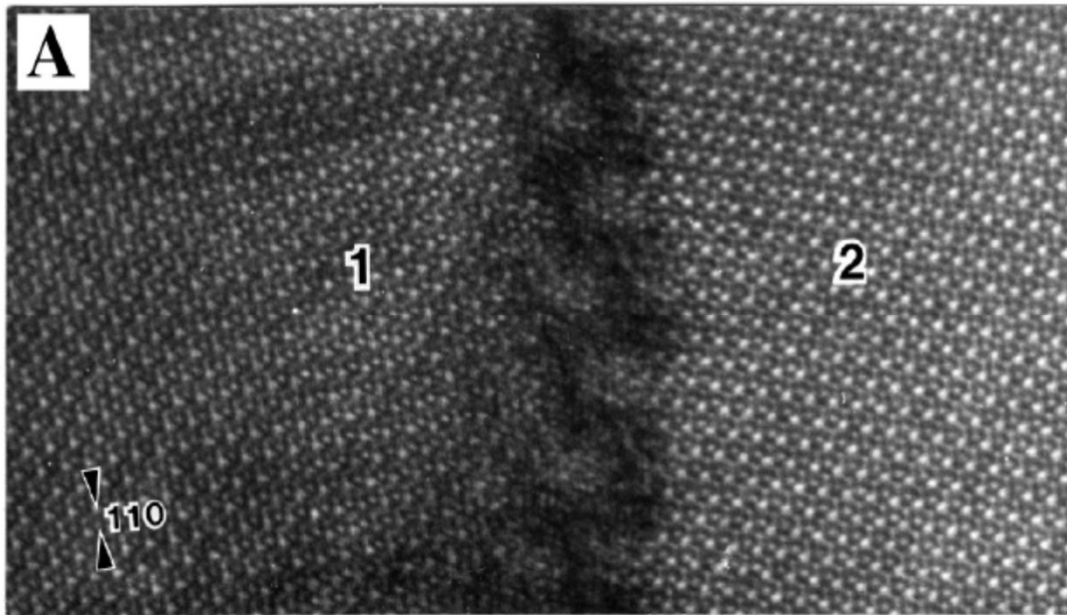
Phase identification

Every crystal has a specific "fingerprint" given by the positions and intensities of the diffraction peaks. The composition of a multi-phase specimen can be determined by fitting its diffraction pattern to the diffraction patterns of pure crystals which can be looked up in a database.

International Centre for Diffraction Data www.icdd.com
550,000 reference materials

Phase transitions, thermal expansion, piezoelectricity, piezomagnetism, bulk modulus, compliance tensor can be measured.

Electron diffraction in a TEM



The wavelength of the electrons is typically much smaller than the lattice spacing. The diffraction peaks in the plane perpendicular to k are observed.

Electron diffraction

In electron diffraction, the intensity of a diffraction peak at reciprocal lattice vector \vec{G} is the square of the structure factor, $n_{\vec{G}}$.

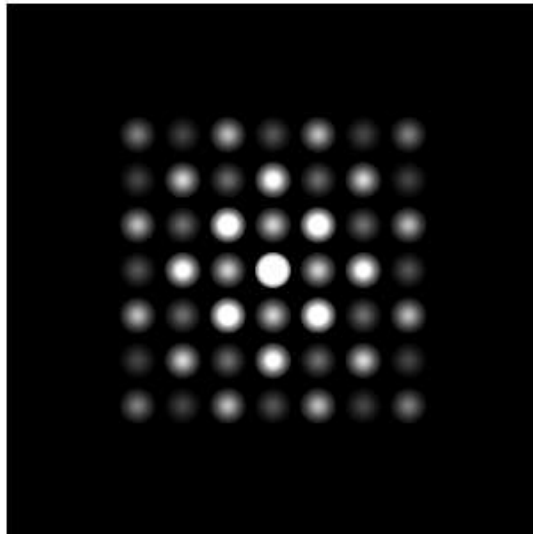
$$n_{\vec{G}} = \frac{1}{V} \sum_j f_j(\vec{G}) e^{-i\vec{G} \cdot \vec{r}_j} = \frac{1}{V} \sum_j f_j(\vec{G}) \left(\cos(\vec{G} \cdot \vec{r}_j) - i \sin(\vec{G} \cdot \vec{r}_j) \right)$$

Here V is the volume of the primitive unit cell, j sums over the atoms in the basis, \vec{r}_j are the positions of the atoms in the basis, and $f_j(\vec{G})$ are the electron atomic form factors evaluated at \vec{G} .

The form below calculates the electron structure factors based on this formula. The crystal structure is specified by providing the primitive lattice vectors and the positions of the atoms in the basis. A basis of up to five atoms can be calculated. The script first calculates the primitive reciprocal lattice vectors and from them calculates the reciprocal lattice vectors $\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$.

On this page, the direction of the incoming electrons is given in terms of the primitive lattice vectors in reciprocal space, $H\vec{b}_1 + K\vec{b}_2 + L\vec{b}_3$. Usually the direction of the incoming electrons are given in terms of the conventional lattice vectors. Be aware that the [100] is a (usually) different direction if primitive lattice vectors are used than if conventional lattice vectors are used.

H: K: L:



[010] →

Primitive lattice vectors:

$$\begin{aligned} \vec{a}_1 &= 4.12\text{E-}10 \hat{x} + 0 \hat{y} + 0 \hat{z} \text{ [m]} \\ \vec{a}_2 &= 0 \hat{x} + 4.12\text{E-}10 \hat{y} + 0 \hat{z} \text{ [m]} \\ \vec{a}_3 &= 0 \hat{x} + 0 \hat{y} + 4.12\text{E-}10 \hat{z} \text{ [m]} \end{aligned}$$

Basis:

The positions of the atoms are given in fractional coordinates between -1 and 1.

Cs	<input type="text" value="0"/>	$\vec{a}_1 +$	<input type="text" value="0"/>	$\vec{a}_2 +$	<input type="text" value="0"/>	\vec{a}_3
Cl	<input type="text" value="0.5"/>	$\vec{a}_1 +$	<input type="text" value="0.5"/>	$\vec{a}_2 +$	<input type="text" value="0.5"/>	\vec{a}_3
<input type="text"/>	<input type="text"/>	$\vec{a}_1 +$	<input type="text"/>	$\vec{a}_2 +$	<input type="text"/>	\vec{a}_3
<input type="text"/>	<input type="text"/>	$\vec{a}_1 +$	<input type="text"/>	$\vec{a}_2 +$	<input type="text"/>	\vec{a}_3
<input type="text"/>	<input type="text"/>	$\vec{a}_1 +$	<input type="text"/>	$\vec{a}_2 +$	<input type="text"/>	\vec{a}_3

Neutron diffraction

Typically a nuclear reactor is used as the neutron source

There are different atomic form factors for neutrons than for x-rays.

Determine the positions of H in biological samples.

Can for example distinguish between Fe and Co which have similar atomic form factors for x-rays.

Structure factor for neutrons

The structure factor for neutrons can be calculated with the following formula,

$$F_{\vec{G}} = \sum_j b_j e^{-i\vec{G}\cdot\vec{r}_j} = \sum_j b_j \left(\cos(\vec{G} \cdot \vec{r}_j) - i \sin(\vec{G} \cdot \vec{r}_j) \right).$$

where \vec{r}_j defines the position of the atom j and \vec{G} is the reciprocal lattice vector. b_j is called the neutron scattering length, it depends on the spin-state of the neutron-nucleus system and the isotope the neutron is scattered from. The scattering lengths can be looked up at the [NIST Center for Neutron Research](http://www.nsl.jrnl.gov/Research/Structure_Factors/).

The form below calculates the neutron structure factors. The script first calculates the reciprocal lattice vectors and from them calculates the reciprocal lattice vectors $\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$. The structure factors are calculated for a few reciprocal lattice vectors and listed in a table.

Primitive lattice vectors:

$\vec{a}_1 =$ $\hat{x} +$ $\hat{y} +$ \hat{z} [m]
 $\vec{a}_2 =$ $\hat{x} +$ $\hat{y} +$ \hat{z} [m]
 $\vec{a}_3 =$ $\hat{x} +$ $\hat{y} +$ \hat{z} [m]

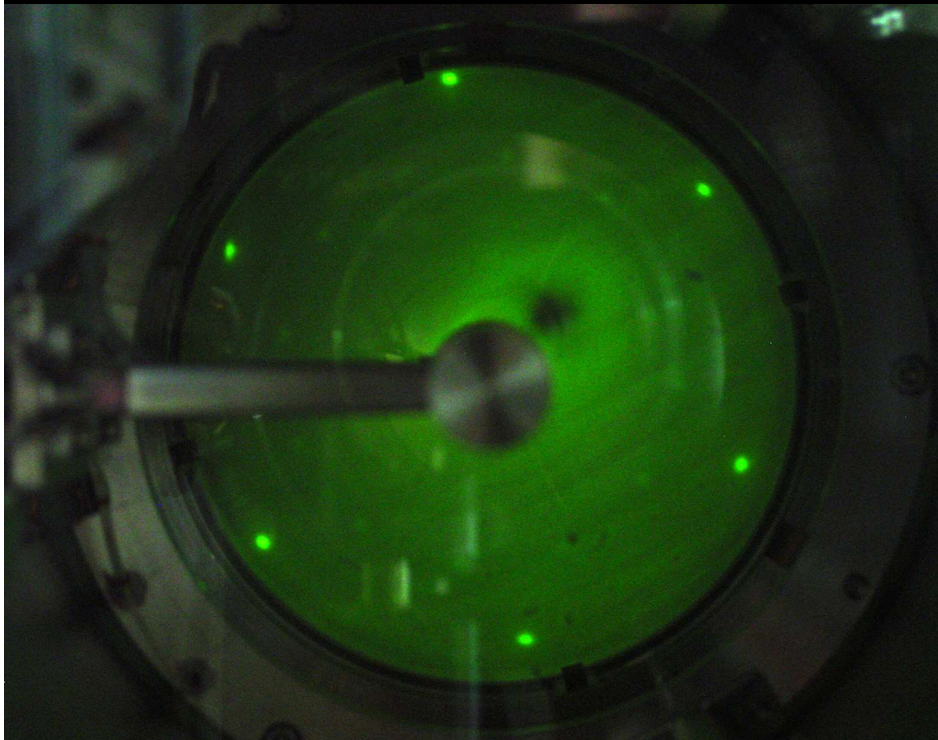
Basis:
 The positions of the atoms are given in fractional coordinates between -1 and 1.

Pb	▼	<input type="text" value="0"/>	$\vec{a}_1 +$	<input type="text" value="0"/>	$\vec{a}_2 +$	<input type="text" value="0"/>	\vec{a}_3
Ti	▼	<input type="text" value="0.5"/>	$\vec{a}_1 +$	<input type="text" value="0.5"/>	$\vec{a}_2 +$	<input type="text" value="0.5"/>	\vec{a}_3
O	▼	<input type="text" value="0"/>	$\vec{a}_1 +$	<input type="text" value="0.5"/>	$\vec{a}_2 +$	<input type="text" value="0.5"/>	\vec{a}_3
O	▼	<input type="text" value="0.5"/>	$\vec{a}_1 +$	<input type="text" value="0"/>	$\vec{a}_2 +$	<input type="text" value="0.5"/>	\vec{a}_3
O	▼	<input type="text" value="0.5"/>	$\vec{a}_1 +$	<input type="text" value="0.5"/>	$\vec{a}_2 +$	<input type="text" value="0"/>	\vec{a}_3
	▼	<input type="text"/>	$\vec{a}_1 +$	<input type="text"/>	$\vec{a}_2 +$	<input type="text"/>	\vec{a}_3
	▼	<input type="text"/>	$\vec{a}_1 +$	<input type="text"/>	$\vec{a}_2 +$	<input type="text"/>	\vec{a}_3
	▼	<input type="text"/>	$\vec{a}_1 +$	<input type="text"/>	$\vec{a}_2 +$	<input type="text"/>	\vec{a}_3

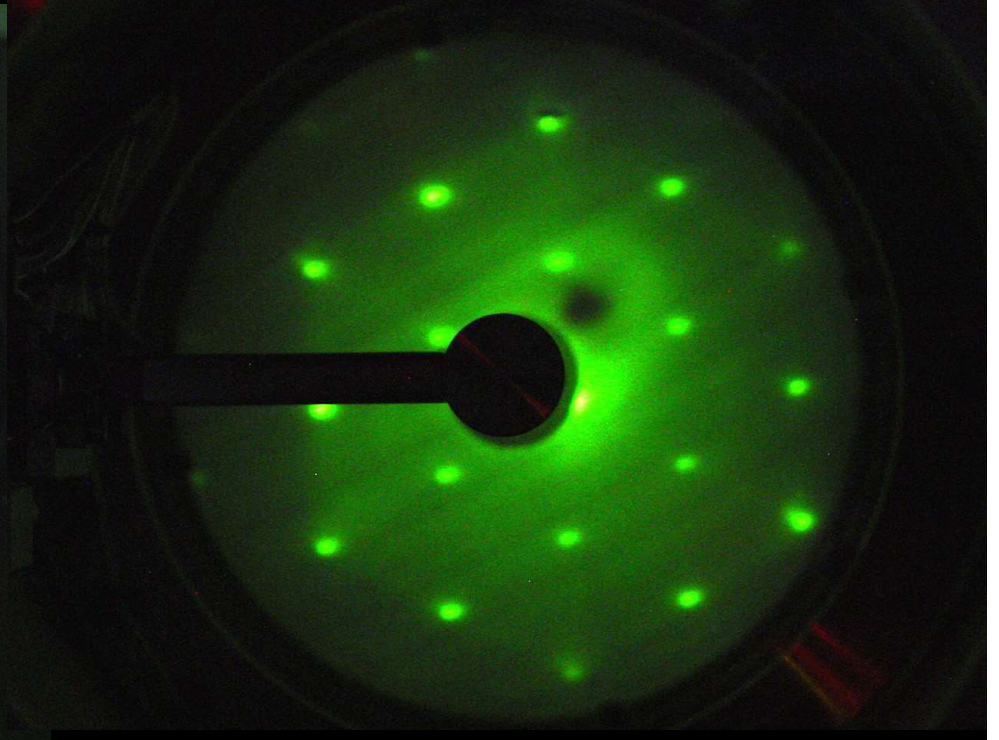
LEED

Low Energy Electron Diffraction

$$100 \text{ V} \rightarrow k \sim 5 \times 10^{10} \text{ m}^{-1}$$



Clean Pd (111)



Pd (111) + 0.3 ML VO_x

LEED is surface sensitive

LEED






Energy of the electron beam: [eV]

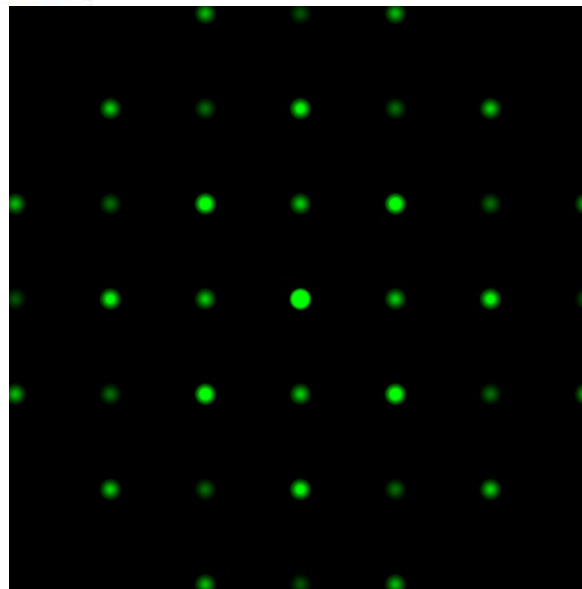
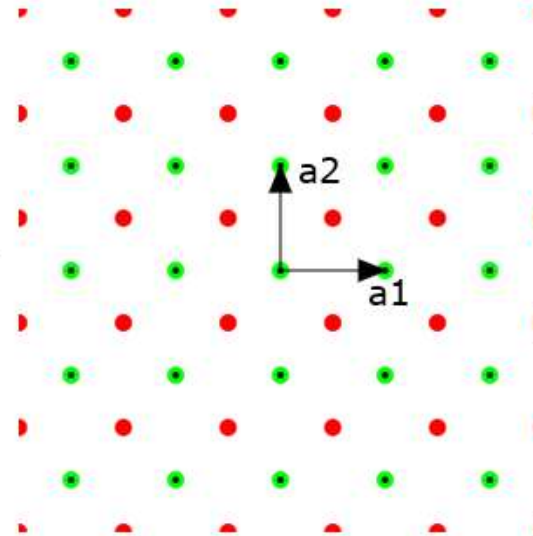
Primitive lattice vectors:

$$\vec{a}_1 = \begin{matrix} 4.12\text{E-}10 & \hat{x} + 0 & \hat{y} \text{ [m]} \\ 0 & \hat{x} + 4.12\text{E-}10 & \hat{y} \text{ [m]} \end{matrix}$$

Basis:

The positions of the atoms are given in fractional coordinates between -1 and 1.

Cs	<input type="text" value="0"/>	$\vec{a}_1 +$	<input type="text" value="0"/>	\vec{a}_2	
Cl	<input type="text" value="0.5"/>	$\vec{a}_1 +$	<input type="text" value="0.5"/>	\vec{a}_2	
	<input type="text"/>	$\vec{a}_1 +$	<input type="text"/>	\vec{a}_2	
	<input type="text"/>	$\vec{a}_1 +$	<input type="text"/>	\vec{a}_2	
	<input type="text"/>	$\vec{a}_1 +$	<input type="text"/>	\vec{a}_2	



Atomic beams

Hydrogen and Helium are used for diffraction studies

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2}$$

Low energies can be used for delicate samples.
Measure the surface like LEED.

Forbidden reflections

Primitive lattice vectors:

$$\vec{a}_1 = 4.12\text{E-}10 \hat{x} + 0 \hat{y} \text{ [m]}$$

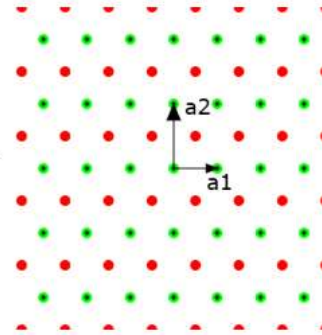
$$\vec{a}_2 = 0 \hat{x} + 6.12\text{E-}10 \hat{y} \text{ [m]}$$

Basis:

The positions of the atoms are given in fractional coordinates between -1 and 1.

C	0	$\vec{a}_1 + 0$	\vec{a}_2	
C	0.5	$\vec{a}_1 + 0.5$	\vec{a}_2	
	0.2	$\vec{a}_1 + 0.3$	\vec{a}_2	
		$\vec{a}_1 +$	\vec{a}_2	
		$\vec{a}_1 +$	\vec{a}_2	

submit



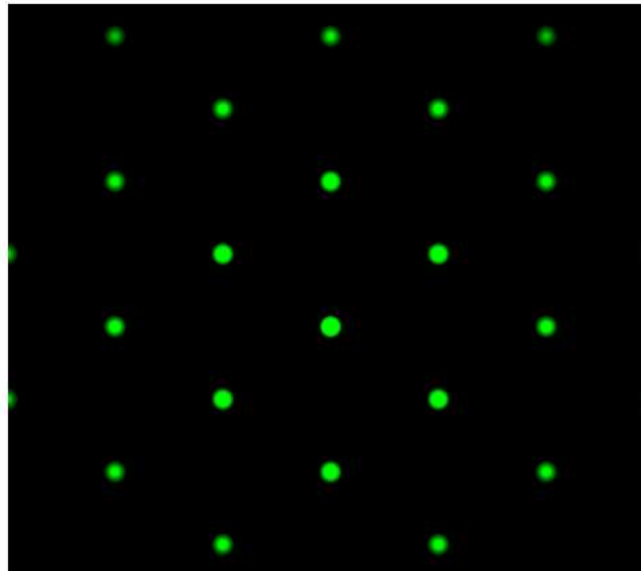
Primitive reciprocal lattice vectors

$$\vec{b}_1 = 2\pi \frac{R \vec{a}_2}{\vec{a}_1 R \vec{a}_2} = 1.525\text{e+}10 \hat{k}_x + 0.000 \hat{k}_y \text{ [m}^{-1}\text{]}$$

$$\vec{b}_2 = 2\pi \frac{R \vec{a}_1}{\vec{a}_1 R \vec{a}_2} = 0.000 \hat{k}_x + -1.027\text{e+}10 \hat{k}_y \text{ [m}^{-1}\text{]}$$

with $R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

Low Energy
Electron Diffraction



Forbidden reflections

$$n_{u.c.}(\vec{r}) = \sum_j Z_j \delta(\vec{r} - \vec{r}_j)$$

Primitive reciprocal lattice vectors

$$\begin{aligned} \vec{b}_1 &= 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 3.939 \hat{k}_x + -2.275e+10 \hat{k}_y + 0.000 \hat{k}_z [\text{m}^{-1}] \\ \vec{b}_2 &= 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 3.939 \hat{k}_x + 2.275 \hat{k}_y + 0.000 \hat{k}_z [\text{m}^{-1}] \\ \vec{b}_3 &= 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 0.000 \hat{k}_x + 0.000 \hat{k}_y + 1.212e+10 \hat{k}_z [\text{m}^{-1}] \end{aligned}$$

$$n_{\vec{G}} = \sum_j Z_j \exp(-i\vec{G} \cdot \vec{r}_j)$$

Structure factors

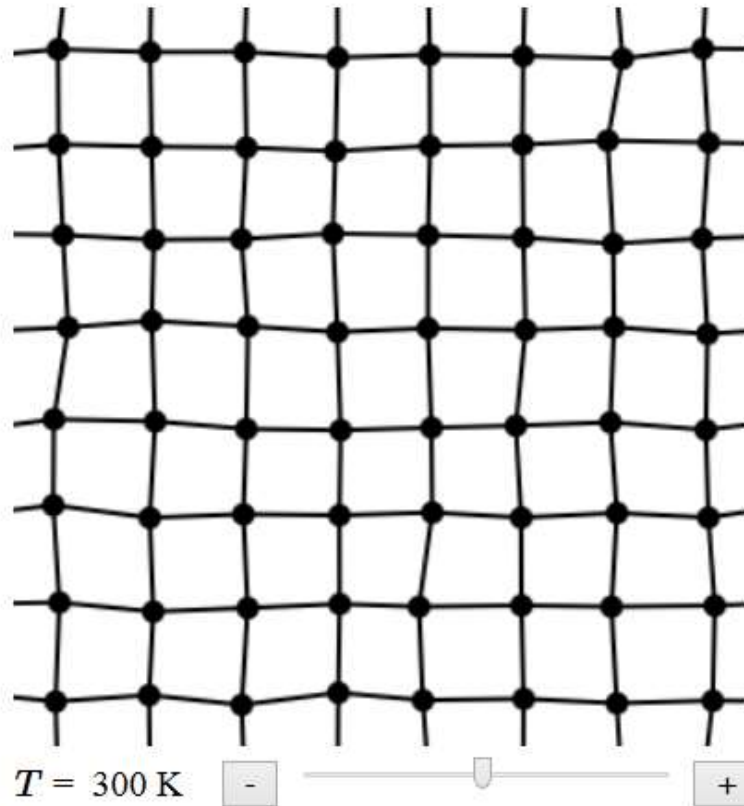
The value of $|n_{\vec{G}}|$ for the 000 diffraction peak is the total number of electrons in the primitive unit cell. The intensities of the peaks in an x-ray diffraction experiment are proportional to $|n_{\vec{G}}|^2$. Note that elements with more electrons produce stronger diffraction intensities.

hkl	$ \vec{G} \text{ \AA}^{-1}$	$ n_{\vec{G}} $	$ n_{\vec{G}} ^2$	$\text{Re}\{n_{\vec{G}}\}$	$\text{Im}\{n_{\vec{G}}\}$
000	0.000	75.94	5767	75.94	0.000
0-10	4.549e-10	37.87	1434	-37.87	0.02201
010	4.549e-10	37.87	1434	-37.87	-0.02201
0-20	9.098e-10	38.17	1457	-38.17	0.04379
020	9.098e-10	38.17	1457	-38.17	-0.04379
0-30	1.365e-9	75.94	5767	75.94	-0.1318
030	1.365e-9	75.94	5767	75.94	0.1318
0-3-1	1.212	0.3909	0.1528	0.02780	0.3899
0-31	1.212	0.3914	0.1532	-0.02727	0.3904
0-2-1	1.212	42.85	1836	-7.648	42.16
0-21	1.212	42.74	1827	7.551	42.07
0-1-1	1.212	43.01	1850	7.610	-42.33
0-11	1.212	42.96	1845	-7.561	-42.29
00-1	1.212	8.896e-8	7.914e-15	-1.573e-8	8.756e-8
001	1.212	8.896e-8	7.914e-15	-1.573e-8	-8.756e-8
01-1	1.212	42.96	1845	-7.561	42.29
011	1.212	43.01	1850	7.610	42.33
02-1	1.212	42.74	1827	7.551	-42.07
021	1.212	42.85	1836	-7.648	-42.16
03-1	1.212	0.3914	0.1532	-0.02727	-0.3904

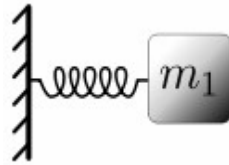
Phonons

Normal Modes and Phonons

At finite temperatures, the atoms in a crystal vibrate. In the simulation below, the atoms move randomly around their equilibrium positions.



Vibrations of a mass on a spring



$$m \frac{d^2 x}{dt^2} = -Cx$$

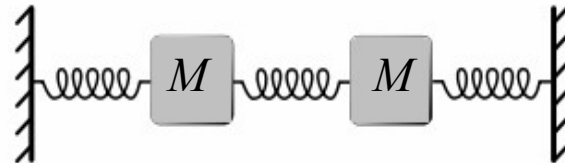
The solution has the form

$$x = Ae^{-i\omega t}$$

$$-\omega^2 mAe^{-i\omega t} = -CAe^{-i\omega t}$$

$$\omega = \sqrt{\frac{C}{m}}$$

Coupled masses



Newton's law

$$M \frac{d^2 x_1}{dt^2} = -Cx_1 + C(x_2 - x_1)$$

$$M \frac{d^2 x_2}{dt^2} = -Cx_2 + C(x_1 - x_2)$$

assume harmonic solutions

$$x_1(t) = A_1 \exp(i\omega t)$$

$$x_2(t) = A_2 \exp(i\omega t)$$

$$-\omega^2 MA_1 e^{i\omega t} = -2CA_1 e^{i\omega t} + CA_2 e^{i\omega t}$$

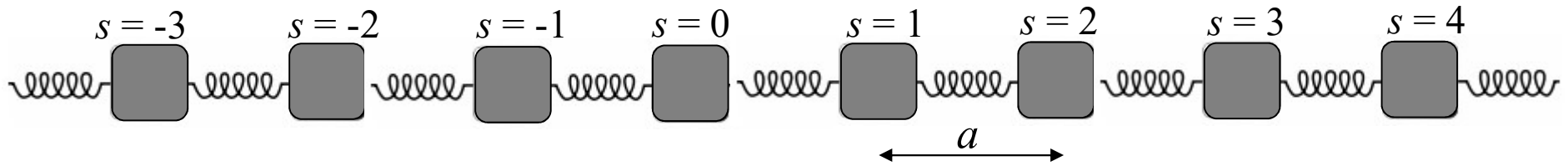
$$-\omega^2 MA_2 e^{i\omega t} = -2CA_2 e^{i\omega t} + CA_1 e^{i\omega t}$$

$$-\omega^2 M \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} -2C & C \\ C & -2C \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$$

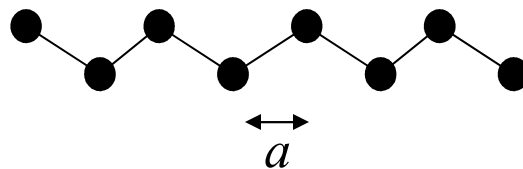
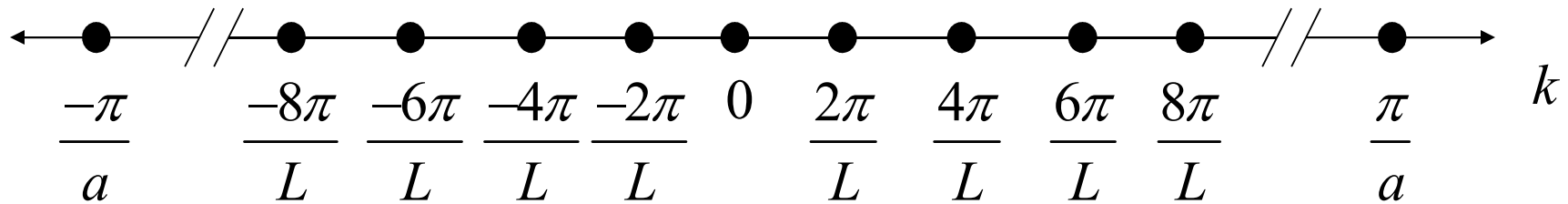
Find the eigenvectors of this matrix

The masses oscillate with the same frequency but different phases

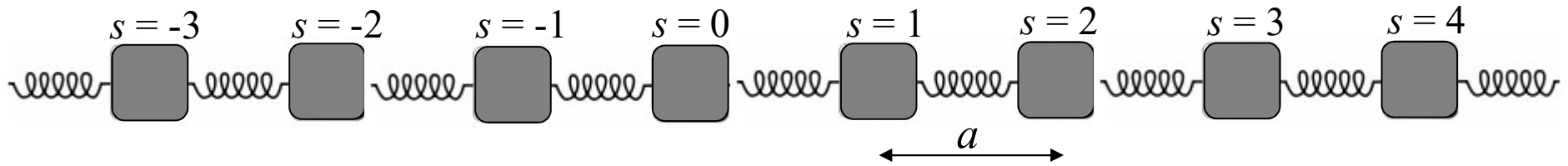
Linear Chain



solution: $u_s = A_k e^{i(ksa - \omega t)} = A_k e^{iksa} e^{-i\omega t}$



Linear Chain



$$m \frac{d^2 u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$$

solutions: $u_s = A_k e^{i(ksa - \omega t)}$

$$-\omega^2 m e^{i(ksa - \omega t)} = C(e^{i(k(s+1)a - \omega t)} - 2e^{i(ksa - \omega t)} + e^{i(k(s-1)a - \omega t)})$$

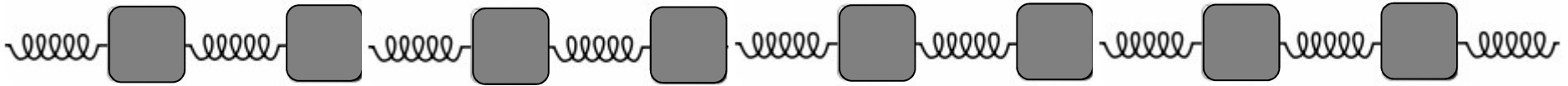
$$-\omega^2 m = C(e^{ika} - 2 + e^{-ika})$$

$$\omega^2 m = 2C(1 - \cos(ka))$$

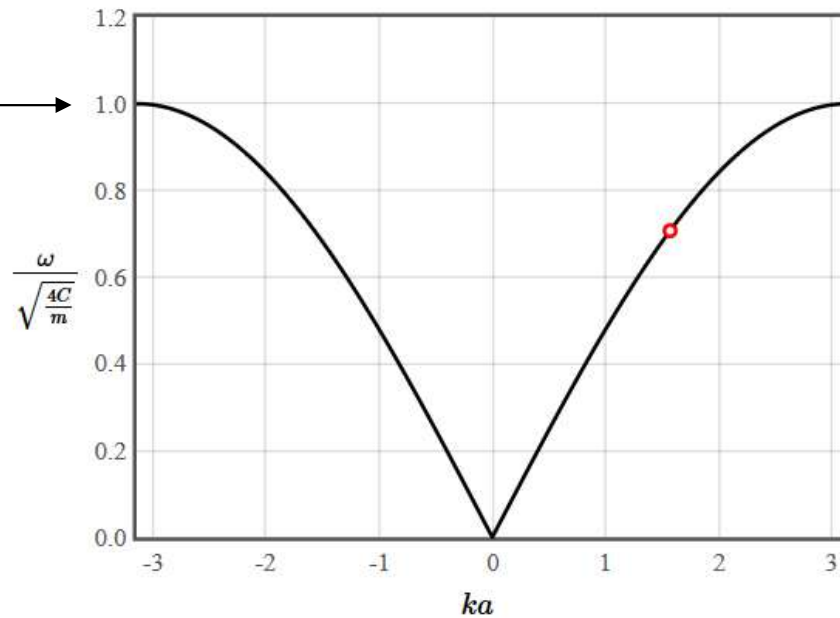
$$\sin^2 \frac{ka}{2} = \frac{1}{2}(1 - \cos ka)$$

$$\omega = \sqrt{\frac{4C}{m}} \left| \sin \left(\frac{ka}{2} \right) \right|$$

Linear Chain - dispersion relation



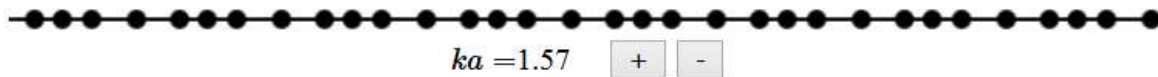
Max. freq. →



$$m \frac{d^2 u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$$

$$u_s = A_k e^{i(ksa - \omega t)}$$

$$\omega = \sqrt{\frac{4C}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

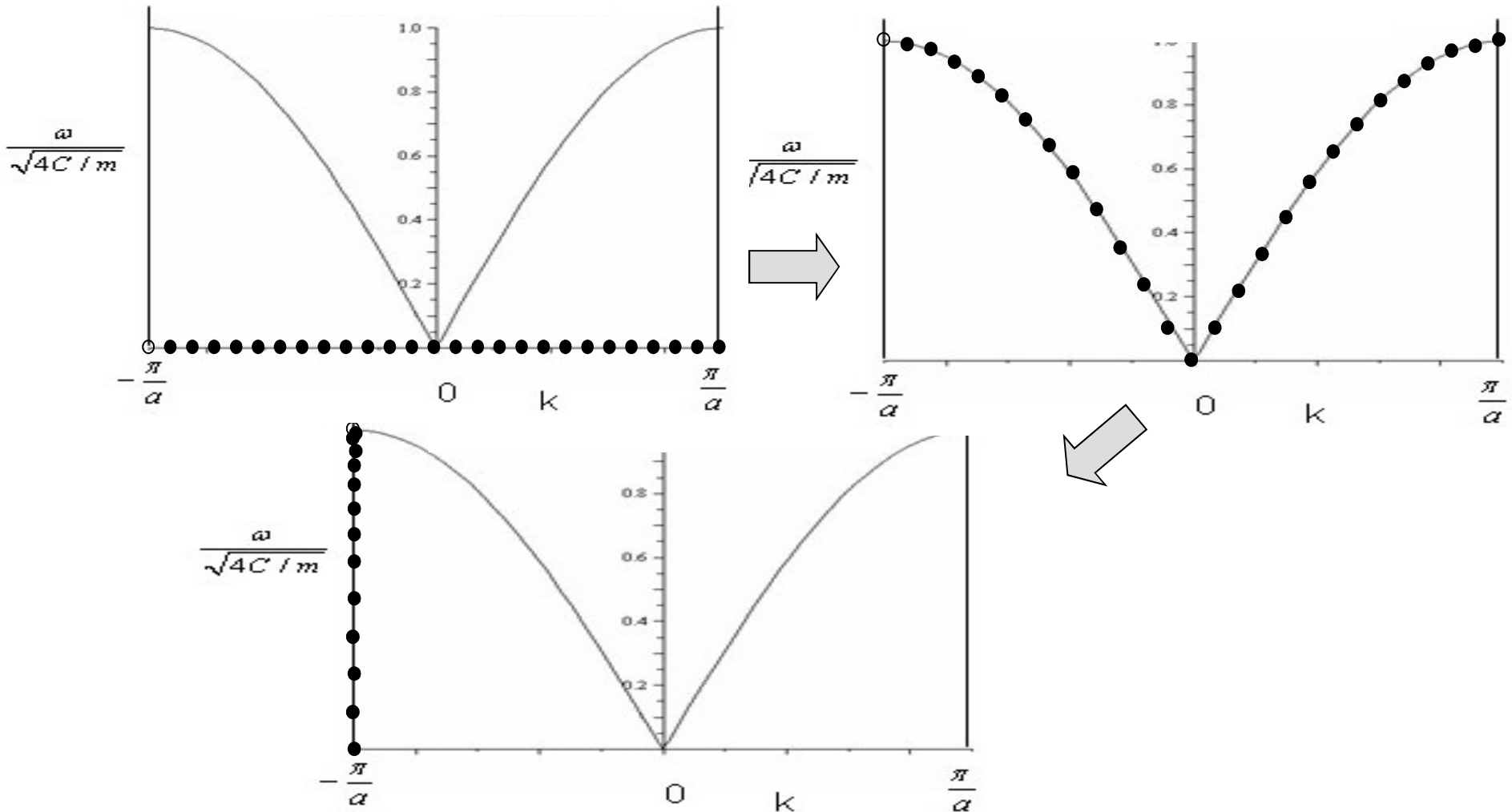


$$\text{speed of sound} = \sqrt{\frac{C}{m}} a$$

Linear Chain - density of states

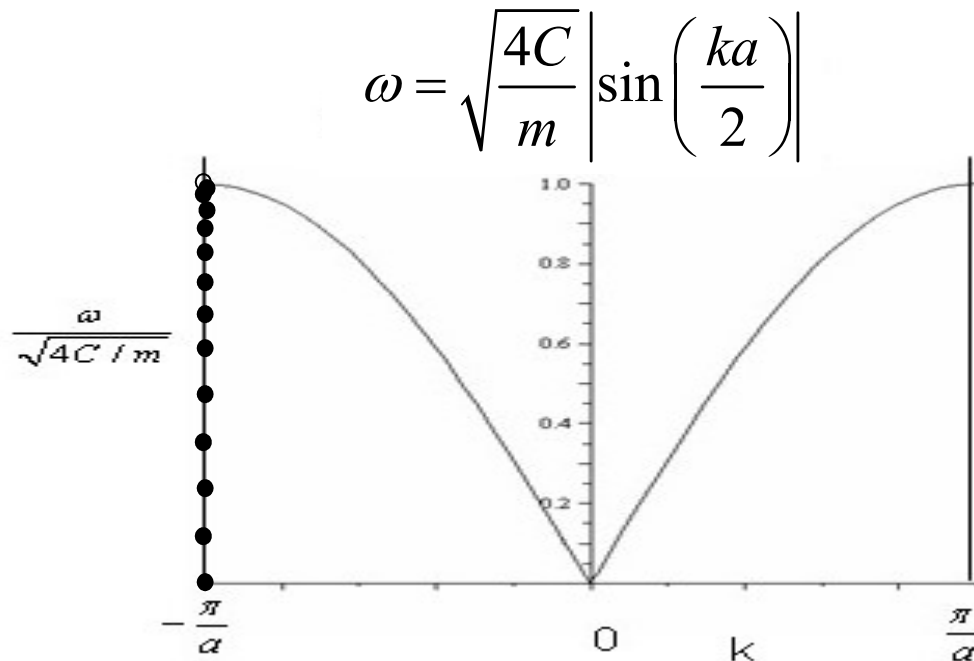
Determine the density of states numerically

$$\omega = \sqrt{\frac{4C}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$



Linear Chain - density of states

This case is an exception where the density of states can be determined analytically.



for every k calculate the frequency

$$\omega = \sqrt{\frac{4C}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

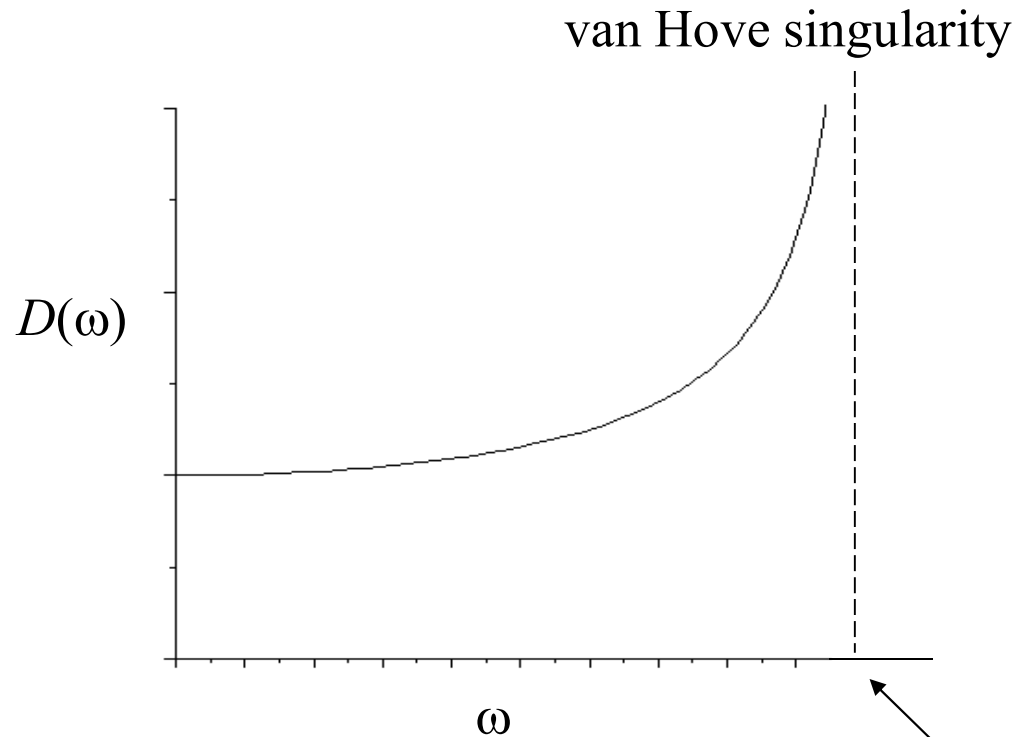
$$D(k) = \frac{1}{\pi}$$

$$D(\omega) = D(k) \frac{dk}{d\omega}$$

$$d\omega = a \sqrt{\frac{C}{m}} \cos\left(\frac{ka}{2}\right) dk$$

$$D(\omega) = \frac{1}{\pi a \sqrt{\frac{C}{m}} \sqrt{1 - \frac{\omega^2 m}{4C}}}$$

density of states



$$\omega = \sqrt{\frac{4C}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

$$D(k) = \frac{1}{\pi}$$

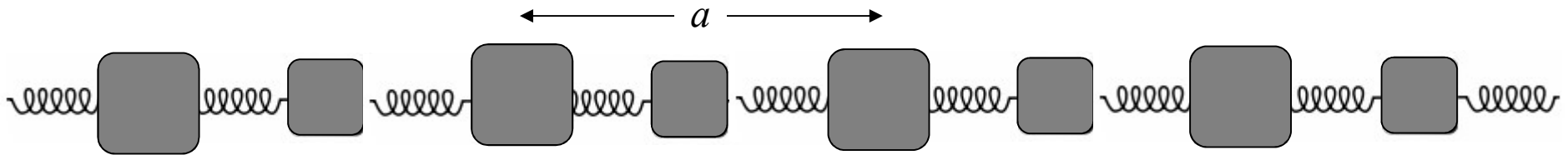
$$D(k)dk = D(\omega)d\omega$$

$$d\omega = a \sqrt{\frac{C}{m}} \cos\left(\frac{ka}{2}\right) dk$$

$$D(\omega) = \frac{1}{\pi a \sqrt{\frac{C}{m}} \sqrt{1 - \frac{\omega^2 m}{4C}}}$$

maximum frequency

Linear chain M_1 and M_2



Newton's law:
$$M_1 \frac{d^2 u_s}{dt^2} = C(v_{s-1} - u_s) + C(v_s - u_s)$$

$2N$ modes
$$M_2 \frac{d^2 v_s}{dt^2} = C(u_s - v_s) + C(u_{s+1} - v_s)$$

assume harmonic
solutions

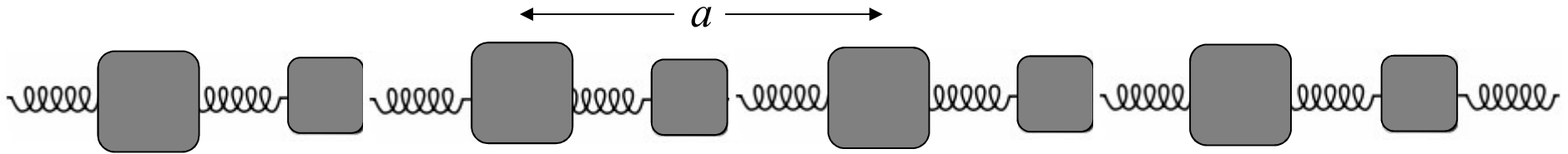
$$u_s = u_k e^{i(ksa - \omega t)}$$

$$v_s = v_k e^{i(ksa - \omega t)}$$

$$-\omega^2 M_1 u_k = C v_k (1 + \exp(-ika)) - 2C u_k$$

$$-\omega^2 M_2 v_k = C u_k (1 + \exp(ika)) - 2C v_k$$

Linear chain M_1 and M_2



$$-\omega^2 M_1 u_k = C v_k (1 + \exp(-ika)) - 2C u_k$$

$$-\omega^2 M_2 v_k = C u_k (1 + \exp(ika)) - 2C v_k$$

$$\begin{bmatrix} \omega^2 M_1 - 2C & C(1 + \exp(-ika)) \\ C(1 + \exp(ika)) & \omega^2 M_2 - 2C \end{bmatrix} \begin{bmatrix} u_k \\ v_k \end{bmatrix} = 0$$

$$M_1 M_2 \omega^4 - 2C(M_1 + M_2) \omega^2 + 2C^2 (1 - \cos(ka)) = 0$$

dispersion relation

$$\omega^2 = C \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm C \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2 \left(\frac{ka}{2} \right)}{M_1 M_2}}$$

Optical phonon branch

$$\frac{\omega}{\sqrt{2C \left(\frac{1}{M_1} + \frac{1}{M_2} \right)}}$$

Acoustic phonon branch

