October 6, 2009

Electronic Materials B Y. Majima	Department	Laboratory	Student ID number	Name
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1-1 Calculate a phase velocity v of plane wave by substituting the wave function $\psi(x) = \psi_0 \exp j(\omega t - k x)$ into the wave equation $\frac{\partial^2 \psi}{\partial t^2} = v^2 \frac{\partial^2 \psi}{\partial x^2}$.

Here, we assume one dimensional plane wave which propagates in x axis direction, where ω is the angular frequency, k is the wave vector.

1-2. When X-ray irradiates a few atomic layers of Au crystals, explain where and how X-ray is scattered in the Au crystal.

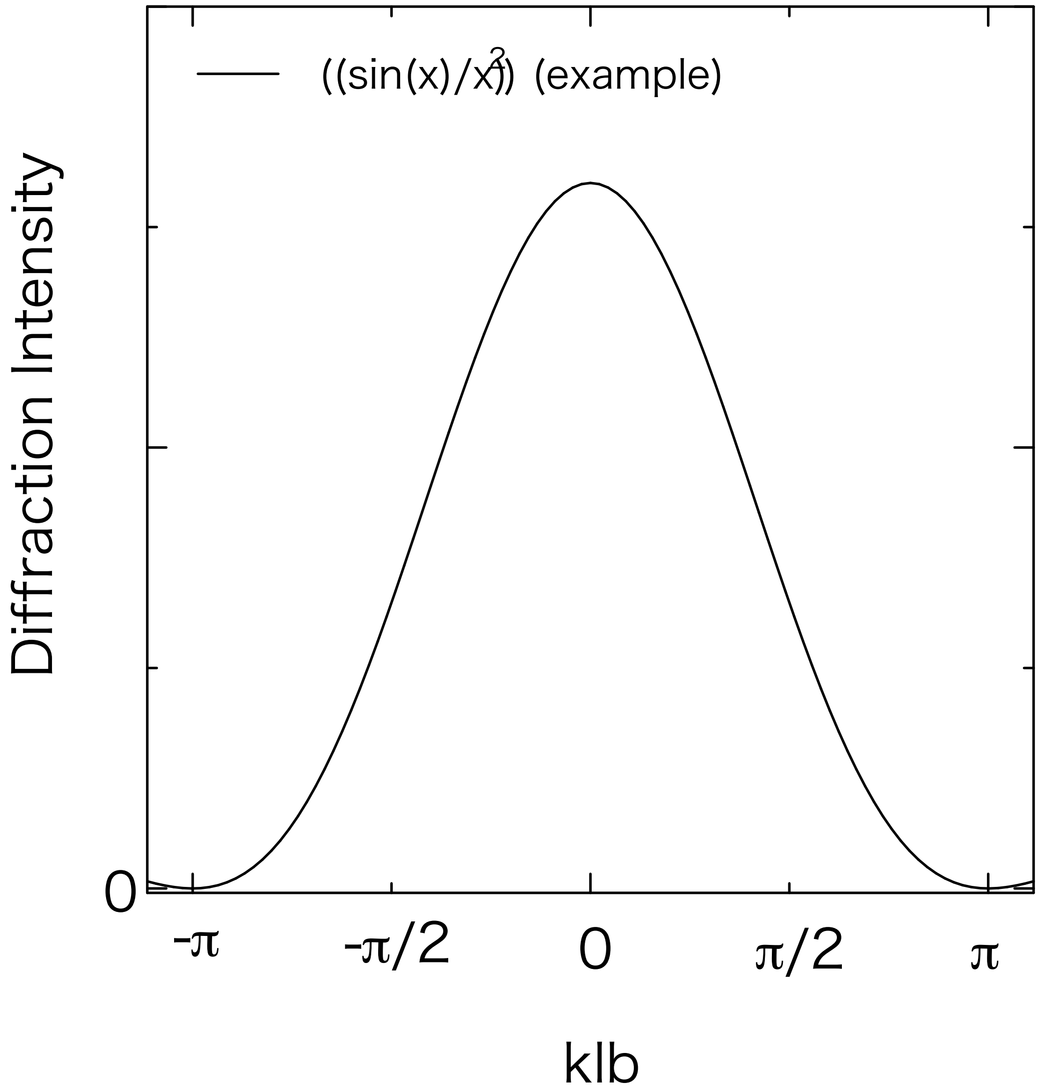
1-3. Diffraction intensity in the diffraction grating (slit width 2b, slit interval d , number of slit N) is given by

$$I = \left(\frac{2b\sin klb}{klb}\right)^2 \left(\frac{\sin\frac{Nkld}{2}}{\sin\frac{kld}{2}}\right)^2,$$

where wavenumber. $k = \frac{2\pi}{\lambda}$ 、$l = \sin\theta$.

Show the *klb* dependence of diffraction intensity in the figure in case of slit width 2*b*, *d*=4*b* and *N*=3.

In the figure below, the Fraunhofer diffraction (*N*=1) intensity with slit width 2b is shown as an example.



No.2 April 10, 2008

Electronic Materials B Y. Majima	Department	Laboratory	Student ID number - -	Name

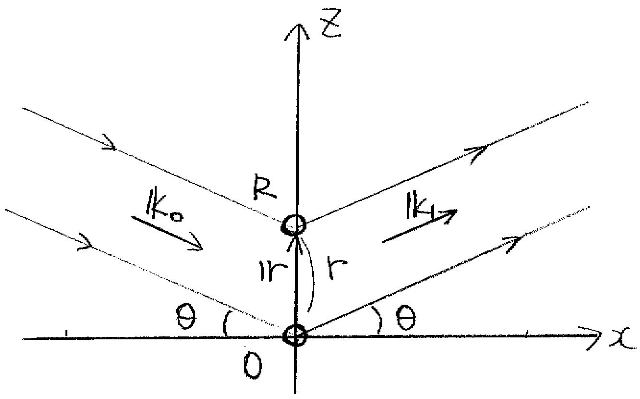
2-1. Why is the value of structure factor $F(\mathbf{k})$ experimentally observed only at scattering vector $\mathbf{k}$ $(= \mathbf{k}_1 - \mathbf{k}_0)$ on the Ewald's sphere of reflection?

2-2. Two atoms exist distance r apart from start point O to point R on z axis as shown in figure.
X-ray is incident where the normal of the wave front is in the z-x plane, the incident angle is measured as θ from x axis and the outgoing angle θ from x axis is as same as incident angle θ.

2-2-1 Give the scattering amplitude G,

2-2-2 Solve the angular dependence of diffraction intensity (I=GG*)

2-2-3 Give the angle where difrraction intensity becomes maximum values.



$\mathbf{k}_0$: wavenumber vector of incidence X-ray

$\mathbf{k}_1$: wavenumber vector of scattered X-ray

$$|\mathbf{k}_0| = |\mathbf{k}_1| = \frac{1}{\lambda}$$

$\mathbf{r}$: positional vector of point R

$$|\mathbf{r}| = r$$

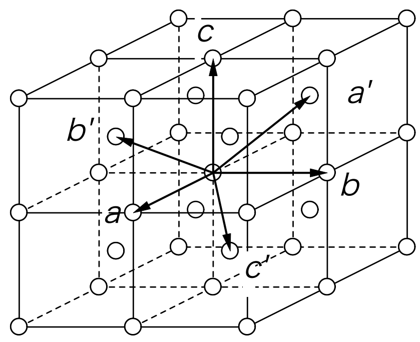
No.3 October 20, 2009

Electronic Materials B Y. Majima	Department	Laboratory	Student ID number - -	Name

3 Answer the following question concerning reciprocal lattice of body-centered cubic (bcc) Bravais lattice and extinction rule of bcc lattice.

Q. 3-1 When we think about the reciprocal lattice of bcc lattice,
the primitive vectors $\mathbf{a}',\mathbf{b}',\mathbf{c}'$ tend to be used rather than orthogonal unit lattice vectors of $\mathbf{a},\mathbf{b},\mathbf{c}$.
Explain the reason why the $\mathbf{a}',\mathbf{b}',\mathbf{c}'$ are used.

Body-centered cubic Bravais lattice



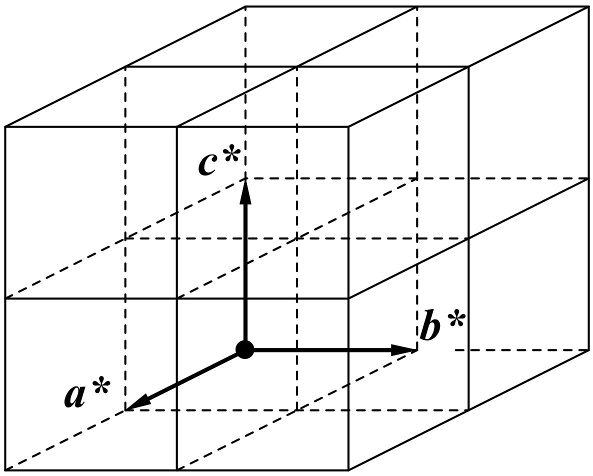
Q. 3-2 Give the reciprocal primitive vector of $\mathbf{a}'^*$ by using fundamental vectors of $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$.
Here, $\mathbf{a} = a\mathbf{x}$, $\mathbf{b} = a\mathbf{y}$, $\mathbf{c} = a\mathbf{z}$, and the size of the vector of the unit lattice is $|\mathbf{a}| = a$,

Q. 3-3 Show the size and direction of the reciprocal primitive vector of $\mathbf{a}'^*$

Q. 3-4 Show the primitive vector of $\mathbf{a}'^*$ on the below figure by using arrow.

Q. 3-5 Show all the reciprocal-lattice points on the below figure by using dots (●).

Reciprocal lattice of body-centered cubic Bravais lattice



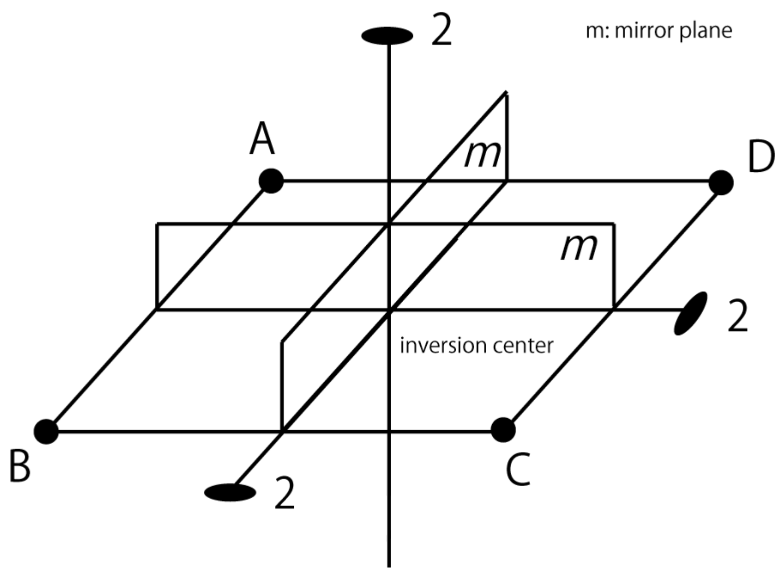
Q. 3-6 Show the structure factor of bcc Bravais lattice by assuming reciprocal lattice vector of $\mathbf{k}(=h\mathbf{a}^*+k\mathbf{b}^*+l\mathbf{c}^*)$ and positional vectors of unit cell atoms of $\mathbf{r}_1=0$, $\mathbf{r}_2=\frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{b}+\frac{1}{2}\mathbf{c}$

Q. 3-7 Explain the extinction rule of bcc Bravais lattice

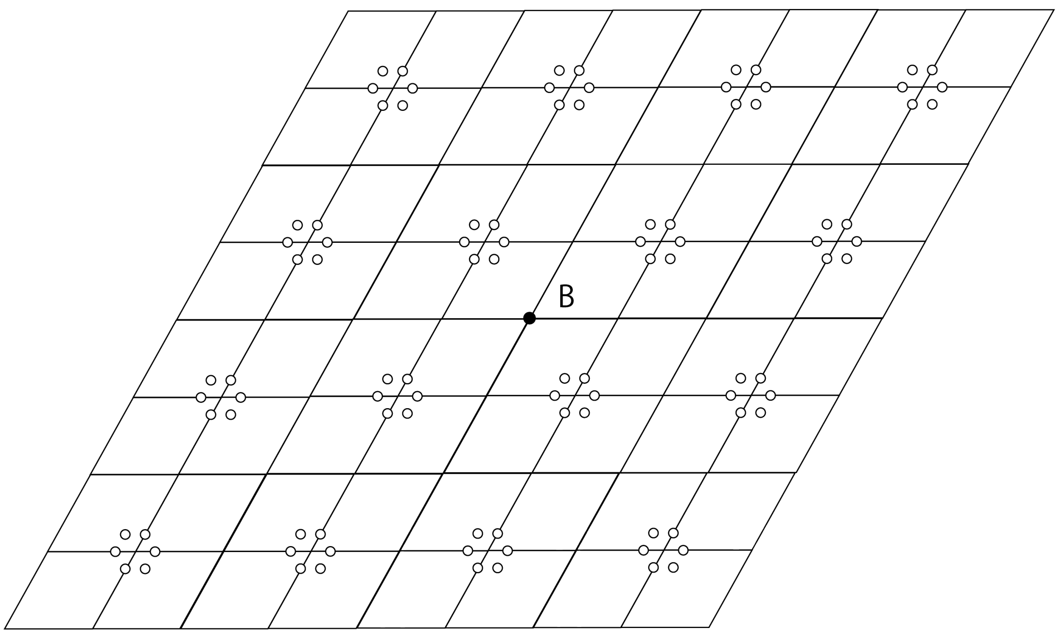
No.4 October 27, 2009

Electronic Materials B Y. Majima	Department	Laboratory	Student ID number - -	Name

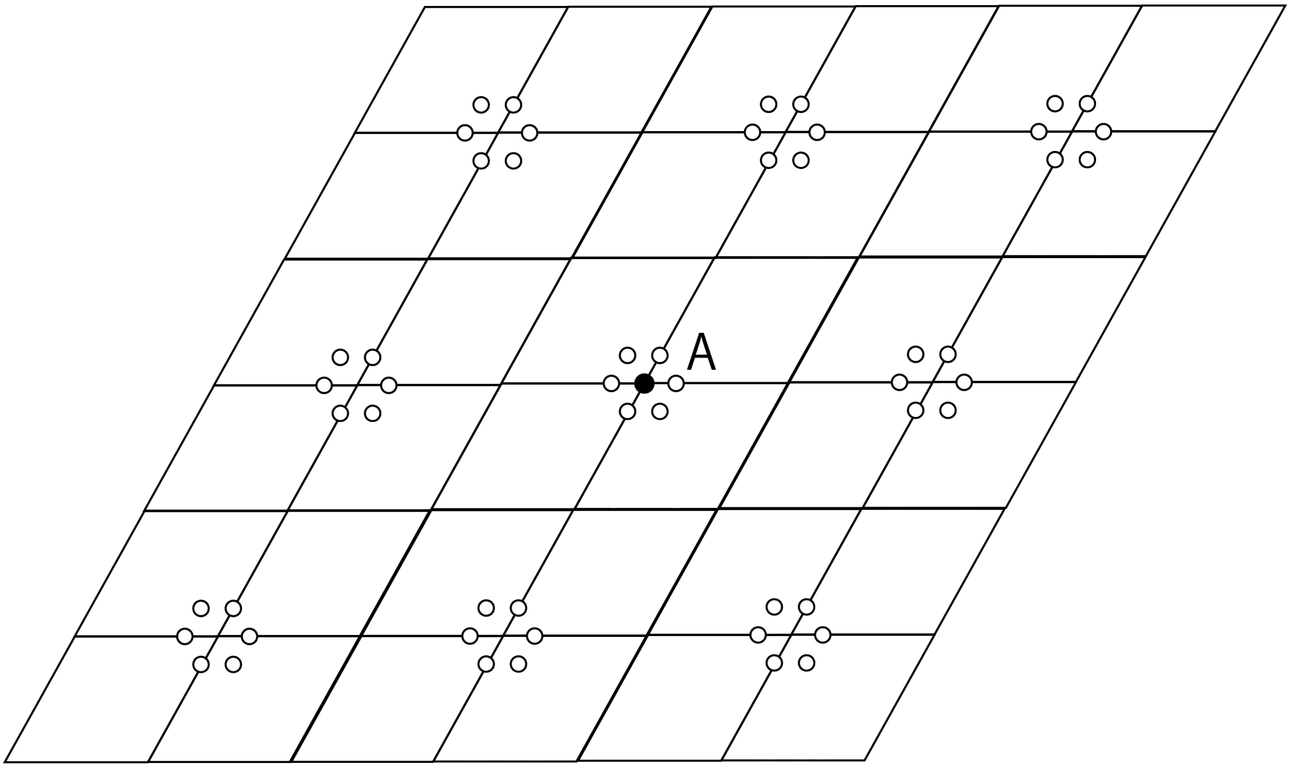
1. Below figure illustrates symmetry elements of a rectangle (a two-dimensional figure). In similar fashion, illustrate all symmetry elements that a square has. [Do not forget rotation-inversion symmetry elements.]



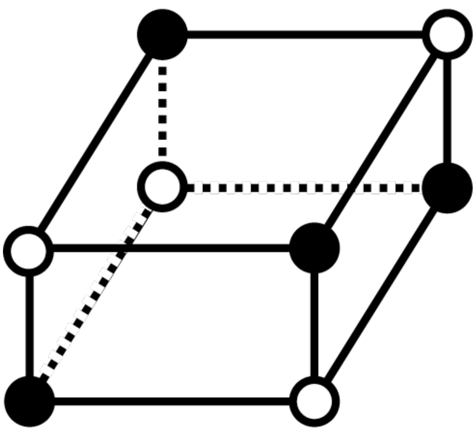
2. What are the symmetry elements around the "false" lattice point B in the figure below? Illustrate the symmetry elements similar as in the previous problem 1. Here, we assume that in the unit cell a=b and γ=60°.

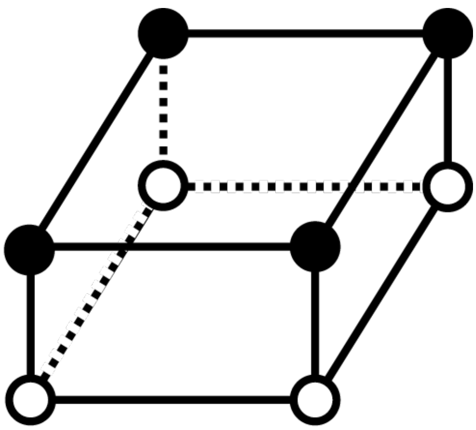


3． What are the symmetry elements around the "true" lattice point A of the two-dimension lattice mentioned in the previous problem 2 (a=b, γ =60°)?
[Hints: Do not forget rotation-inversion symmetry.]



4． Black and white spheres are placed on the corners of a quadratic prism (a=b≠c, $\alpha = \beta = \gamma$ =90°). Illustrate the symmetry elements of the quadratic prism, similar as in the previous problem 1.





No.5 November 4, 2009

Electronic Materials B Y. Majima	Department	Laboratory	Student ID number	Name
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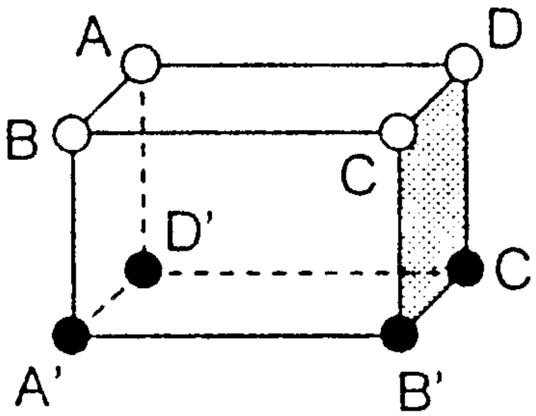
1. What is the product of C_3^2 and σ^c $(\sigma^c C_3^2)$? Find the answer by actually operating the elements successively (first C_3^2 and then σ^c) to the regular triangle lmn.

2. Two kinds of atoms, represented by closed and open circles, are placed on the corners of a rectangular parallel piped, as shown in right figure.

2-1 What are the symmetry elements for this system?



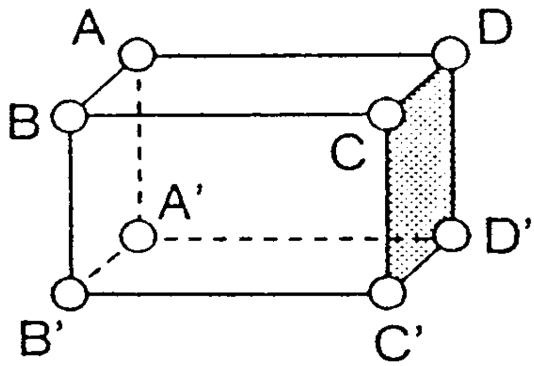
2-2 Draw the stereographic projection of the symmetry elements.

2-3 What point group do these elements form?

2-4 What is the order of the point group?

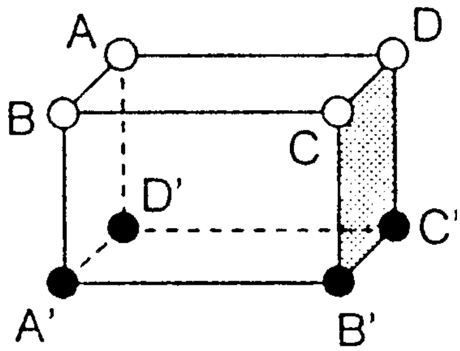
2-5 Draw the $\bar{2}$ axis. And show the relation between the $\bar{2}$ axis and its associated mirror plane.

2-6 The atoms are placed on the corners as shown in right figure.
What point group do these symmetry elements form?
Draw the stereographic projection of the point group.



3. On the symmetry elements for the system shown in right figure,

3-1 Draw the multiplication table.



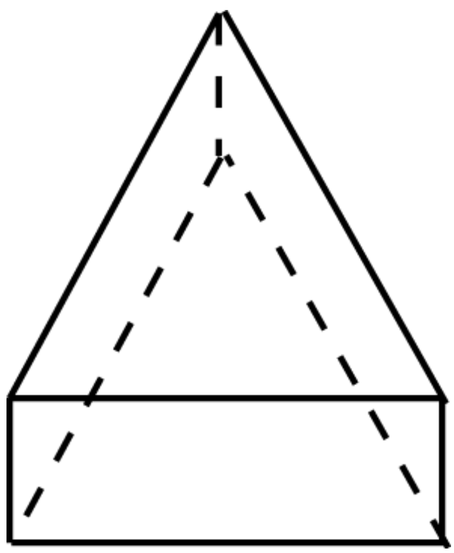
3-2 Check that the elements form a group.

3-3 Find the sub-groups of the group.

3-4 Show the generating elements of the group.

4. The symmetry elements for a regular triangular prism (right figure) forms the point group D_{3h} ($\bar{6}2m$).

Show the symmetry elements for this point group, similar as in Question 1 in the last Exercise.



No.6 November 10, 2008

Electronic Materials B Y. Majima	Department	Laboratory	Student ID number	Name
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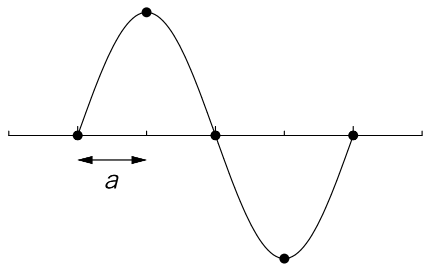
6-1. In a liner chain of monatomic Bravais lattice, consider a dispersion of angular frequency ω_k against wavenumber k of $\omega_k = 2\sqrt{\frac{\alpha}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$.

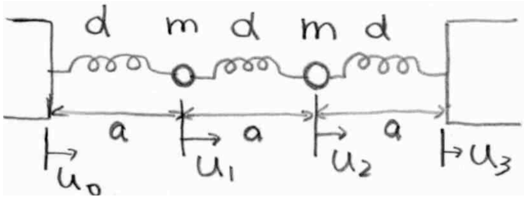
Q6-1-1 Calculate k when ω_k becomes maximum ($\omega_k^{\max}$), and show corresponding lattice vibration mode by referring the right figure.
Here the closed circles show the lattice points (atom) and the z-axe shows the displacement.



Q6-1-2 Calculate k when ω_k becomes $\frac{\omega_k^{\max}}{\sqrt{2}}$, and show the corresponding lattice vibration mode by referring the above figure.

6-2. Consider the normal modes of a one-dimensional Bravais lattice with two atoms that fixed at the ends, with equilibrium positions of a and $2a$.

Here we assume the linear chain of identical two atoms (mass m), connected by spring strength of α, and the displacements of the first and the second atoms as u_1 and u_2, respectively.



(This problem is a part of the end-of-term examination, 2005)

6-2-1. Calculate the harmonic potential energy U

6-2-2. Calculate the equations of motion of each first and second atoms by using u_1, u_2, m, α.

6-2-3. Calculate wavenumber k and explain the relationship between A_k and B_k by substituting boundary condition of $u_0 = u_3 = 0$ into $u_l = (A_k \exp(ikla) + B_k \exp(-ikla))\exp(-i\omega_k t)$ where ω_k is angular frequency.

6-2-4. Calculate u_1 and u_2.

6-2-5. Calculate all eigenfrequencies ω_k, and explain those fundamental vibration modes.

No.7 December 8, 2009

Electronic Materials B Y. Majima	Department	Laboratory	Student ID number	Name
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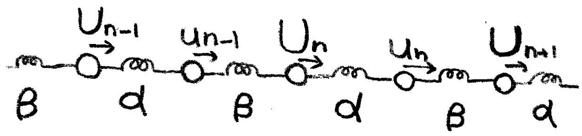
7. Consider normal modes of a one-dimensional Bravais lattice with two atoms (mass m) per primitive cell in which the two atoms are connected by the two springs alternatively (spring constants α, β).

Here, U_n: displacement of the atom (mass m) that oscillates about the site na,

u_n: displacement of the atom (mass m) that oscillates about the site $(n+\frac{1}{2})a$, and



assuming $U_n = A_U \exp\lfloor i(kna - \omega\ t)\rfloor$、$u_n = A_u \exp\lfloor i(kna - \omega\ t)\rfloor$.

Q7-1 Give the equation of motion at U_n and u_n.

Q7-2 Solve the two branches of ω_+ and ω_-.

Q7-3 Explain the two mode of vibration under the case of $\alpha > \beta$ at $k = \frac{\pi}{a}$.

Q7-4 Explain the two mode of vibration under the case of $\alpha > \beta$ at $k \to 0$.