

## Lattice with 2 atoms per primitive cell

1. Let's look at a plane that contains only one kind of atom (say the 100 plane in the SC lattice of CsCl, or the 111 plane in the FCC lattice of NaCl both of which contain only one kind of atom). Let's call the displacement from its equilibrium position of this plane,  $u_s$ . Let's call the displacement from its equilibrium position of the next plane which contains only the other kind of atom,  $v_s$ .

2. Let's **consider only nearest neighbor interactions**, and call the spring constant between these  $C_{12} = C$ . Let's also call the mass of the one atom,  $M_1$ , and the mass of the other atom,  $M_2$ , where  $M_1 > M_2$ . (Cl has a mass of 35.4 amu; Na has a mass of 23.0 amu; Cs has a mass of 132.9 amu.)

Note: If we put one kind of atom at a lattice point and the other in the hole, we have the same kind of lattice if we consider the other atom as at the lattice point and the first atom in the hole. In other words, it doesn't matter if we put the Cl atom at the lattice point and Na in the hole, or put CS at the lattice point and Cl in the hole.

3. Since we have **two** different atoms, we will have **two** different equations from **Newton's Second Law**:

$$\begin{aligned} M_1 d^2u_s/dt^2 &= C(v_s - u_s) + C(v_{s-1} - u_s), \quad \text{and} \\ M_2 d^2v_s/dt^2 &= C(u_{s+1} - v_s) + C(u_s - v_s). \end{aligned}$$

4. Let's try a solution similar to that for the monatomic lattice:

$$\text{guess: } u_s = u_0 e^{iKsa} e^{i\Omega t}, \quad \text{and} \quad v_s = v_0 e^{iKsa} e^{i\Omega t}.$$

We now simply substitute these guesses into both of the differential equations (Newton's Second Law) and see if we get solutions (that is, the equations hold):

$$\begin{aligned} -M_1 \Omega^2 u_0 &= C v_0 (1 + e^{-iKa}) - 2C u_0, \quad \text{and} \\ -M_2 \Omega^2 v_0 &= C u_0 (1 + e^{+iKa}) - 2C v_0; \end{aligned}$$

or simplifying:

$$\begin{aligned} (2C - M_1 \Omega^2) u_0 - C(1 + e^{-iKa}) v_0 &= 0, \quad \text{and} \\ (2C - M_2 \Omega^2) v_0 - C(1 + e^{+iKa}) u_0 &= 0. \end{aligned}$$

One answer would be that  $u_0 = 0 = v_0$ , but this simply says that there is no oscillation - a trivial solution.

5. This is a system of **two equations in two unknowns**. For a non-trivial solution to exist, the determinate of the coefficients of  $u_0$  and  $v_0$  must be equal to zero. {That is, if  $ax+by=0$  and  $cx+dy=0$ , then there is a non-trivial solution only if  $ad-bc=0$ .} [Alternately, solve for  $y$  in terms of  $x$ :  $y=-cx/d$ ; then substitute this into the other equation:  $ax + b(-cx/d) = 0$  to get  $(a-bc/d)x = 0$ , so if  $x \neq 0$  then  $ad-bc=0$ .]

$$\Omega^2 = \{ 2C(M_1+M_2) \pm [ 4C^2(M_1+M_2)^2 - 4M_1M_2(2C^2)(1-\cos(Ka)) ]^{1/2} \} / 2M_1M_2.$$

Note that this is the **dispersion relation** as it gives  $\Omega(K)$ .

Note that there is a  $\pm$  in the expression. This indicates that there are **TWO K's for each  $\Omega$** .

We interpret this to mean that there are **two branches**, or modes, of oscillation for a diatomic lattice.

It is your job in **homework problem 14** parts b and c to see what the dispersion relation looks like near  $K=0$  and near  $K=1/2G$  (that is,  $Ka=\pi$ ).

6. From the **case where K is near zero**, we get (you get from doing *homework problem 14*, part b) that one solution gives you:

$$\Omega_- = [C/\{2(M_1+M_2)\}]^{1/2} a K \quad (\text{which says } \Omega_- \propto K, \text{ so } v_{\text{phase}} = v_{\text{group}} = \text{constant}), \text{ and}$$

$$\Omega_+ = [2C\{(1/M_1)+(1/M_2)\}]^{1/2} \quad (\text{which says } \Omega_+ \approx \text{constant so } v_{\text{group}} \approx 0).$$

**Substituting the  $\Omega_-$**  expression into either of our two equations (say the first one):

$$(2C - M_1\Omega_-^2)u_0 - C(1 + e^{-iKa})v_0 = 0, \quad \text{or, with } \Omega_- \approx 0 \text{ when } K \approx 0:$$

$$2Cu_0 - C(1+1)v_0 = 0, \quad \text{or } \mathbf{u_0 = v_0},$$

that is, that the amplitudes of u and v are approximately equal.

**Substituting the  $\Omega_+$**  expression into either of our two equations (say the first one):

$$(2C - M_1\Omega_+^2)u_0 - C(1 + e^{-iKa})v_0 = 0,$$

or with  $\Omega_+ \approx [2C\{(1/M_1 + 1/M_2)\}]^{1/2}$  when  $Ka \approx 0$ :

$$(2C - M_1[2C\{(1/M_1 + 1/M_2)\}])u_0 - C(1 + 1)v_0 = 0, \quad \text{or}$$

$$\mathbf{-(M_1/M_2)u_0 = v_0},$$

that is, that the oscillations of u and v are 180° out of phase and that u and v oscillate about the center of mass.

We now name these two branches according to their oscillations. The oscillations that are **IN PHASE** we call the **acoustical mode**, and the oscillations that are **OUT OF PHASE** we call the **optical mode**. These names come from the fact that the acoustical refers only to the motion of the masses, while the optical refers to the fact that the different atoms are really different ions (one positive, one negative) and so will oscillate out of phase with any electromagnetic wave (light-optic).

[In 3-D for p atoms, there will be 3 acoustical modes and 3p-3 optical modes.]

7. Completing the  $\Omega$  vs K diagram we note (from *homework problem 14*, part c) ) that the

**acoustical mode** (using the negative sign in the dispersion relation) goes

from  $\Omega \approx 0$  for  $K \approx 0$  up to  $\Omega \approx [2C/M_1]^{1/2}$  for  $K \approx \pi/a$ ,

while the **optical mode** (using the positive sign in the dispersion relation) goes from

$\Omega \approx [2C\{(1/M_1)+(1/M_2)\}]^{1/2}$  for  $K \approx 0$  down to  $\Omega \approx [2C/M_2]^{1/2}$  for  $K \approx \pi/a$ .

This indicates that [since  $M_1 > M_2$ ,  $(1/M_1) < (1/M_2)$ ] there is a **GAP in values of  $\Omega$  for which there are no real K values**. If we substitute this  $\Omega$  (for which there are no real values of K, only complex ones) into our equations for  $u_s$  and  $v_s$ , we get exponential decay as our solution. This indicates that **this frequency cannot propagate into the crystal**.

