VIBRATIONAL DYNAMICS OF ATOMS IN A ONE-DIMENSIONAL CRYSTAL LATTICE

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ABSTRACT

A crystal is composed of a periodic arrangement of atoms and molecules that vibrate around their equilibrium positions due to thermal motion at finite temperatures. When atoms are displaced from these positions, they experience a restoring force that follows Hooke's law and is proportional to the displacement. This study analyzes the vibrational dynamics of a one-dimensional lattice, where the atoms are modeled as masses connected by springs with a force constant. The motion of atoms in this system is governed by the equations of motion, and the resulting lattice vibrations are examined in the context of phase velocity, sound velocity, and Brillouin zones. The analysis is further extended to a lattice consisting of two different kinds of atoms, leading to the formation of distinct acoustic and optical modes. The dispersion relations and the role of wave vectors defined by cyclic boundary conditions are explored, with emphasis on the periodic nature of the ω-q curve and the significance of the first Brillouin zone.

Keywords: *Crystal lattice, lattice vibrations, Hooke's law, one-dimensional lattice, phase velocity, sound velocity, Brillouin zone, dispersion relation, wave vector, cyclic boundary conditions, acoustic mode, optical mode.*

INTRODUCTION

A crystal consists of a periodic arrangement of atoms and molecules. However, the atoms or molecules of a crystal vibrate around the equilibrium positions at finite temperatures because of their thermal motion. When a atom is displaced from its equilibrium position, the atom is subject to a restorating force depending on the displacement. The restorating force follows Hooke's law and is proportional to the displacement. When each atom vibrates randomly, each atom suffers random forces and its vibration is immediately damped. On the other hand, if each atom vibrates with a small relative displacement from the neighboring atoms, then the vibration will

continue with its small vibration energy. For simplicity we consider the one-dimensional lattice shown in Fig.1, where the mass of the atoms is M and the distance between the nearest neighbor atoms (lattice constant) at equilibrium is a. We assume that the interatomic forces act on neighboring atoms only and that the atoms are connected to each other by a spring constant (force constant) k_0. Defining the displacement of the atoms from their equilibrium positions by u_0, u_1, u_2 , $\cdots, u_n, u_{n+1}, \cdots$, the equation of motion of nth atom

$$M\frac{\mathrm{d}^2}{\mathrm{d}t^2}u_n = -k_0(u_n - u_{n-1}) - k_0(u_n - u_{n+1}) \tag{1}$$

As stated above, when the displacement of each atom is independent, an atom will be subject to a strong force from the neighboring atoms and the

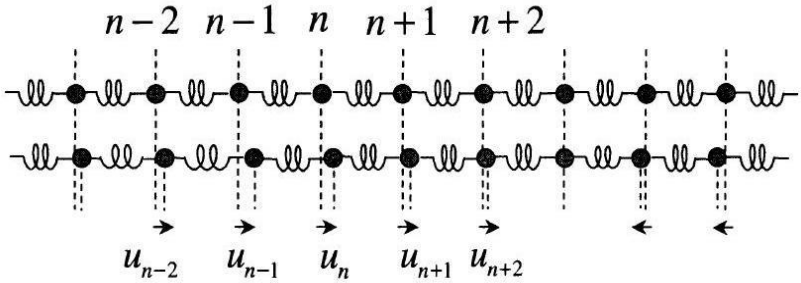

Fig. 1. Displacement of atoms from their equilibrium positions (lattice vibration) displacement is damped. Therefore the lowest excitation energy of the lattice vibration corresponds to a wavelike displacement, keeping the displacement of neighboring atoms almost in phase, when we see neighboring atoms. In such a case we may write the solution of (1) as

$$u_n = A\exp[\mathrm{i}(qna - \omega t)] \tag{2}$$

where $q = \omega/v_s = 2\pi/\lambda$ is the wave vector, ω is the angular frequency, v_s is the velocity of sound, and λ is wavelength. Inserting (2) into (1), we obtain

$$M\omega^2 = -k_0\left(\mathrm{e}^{\mathrm{i}qa} + \mathrm{e}^{-\mathrm{i}qa} - 2\right) = 4k_0\sin^2\left(\frac{qa}{2}\right) \tag{3}$$

From this we have following relation:

$$\omega = 2\sqrt{\frac{k_0}{M}}\left|\sin\left(\frac{qa}{2}\right)\right| \tag{4}$$

When the wavelength is much longer than the lattice constant $(qa \ll 1)$, the phase velocity v_s is given by

$$v_s = \frac{\omega}{q} = \sqrt{\frac{k_0}{M}}a\frac{\sin(qa/2)}{(qa/2)} \cong \sqrt{\frac{k_0}{M}}a \ (qa \ll 1) \tag{5}$$

METHODS

This result indicates that a lattice vibration with long wavelength has a constant phase velocity $v_s = \sqrt{k_0/M}a$, which corresponds to the sound velocity. Figure 2 shows the calculated curve from (4), where we see that the $\omega - q$ curve is a periodic function with a period of $2\pi/a$. The whole dispersion curve is the repetition or displacement of the curve in the period $-\pi/a \leq q \leq \pi/a$, and thus this feature enables us to discuss lattice vibrations in that period. The region of the period is called the first Brillouin zone, and the second Brillouin zone is shown in Fig. 2. The second, third and other Brillouin zones are equivalent to the first Brillouin zone, which is shown in Sect. 1.4 in detail in connection with the reduced zone scheme. Where there are N atoms, N degrees of freedom of motion exist. Adopting cyclic boundary conditions we can define wave vectors by $q = 2\pi n/(Na)$, where $n = (-N/2 + 1) \sim (+N/2)$, giving rise to N values of the wave vectors. The above defined wave vectors are obtained from the cyclic boundary condition such that the displacement u_n of (2) is equivalent for $n = 0$ and $n = N$.

Next, we consider a lattice consisting of two kinds of atoms with masses M_1 and M_2. The atomic distance of the atoms of mass M_1 is a and the same is true for the atoms M_2. When the nearest-neighbor interaction is assumed, the equations of motion are written as in the case of the one-dimensional lattice stated above as

$$\left.\begin{aligned} M_1 \frac{\mathrm{d}^2}{\mathrm{d}t^2} u_{2n+1} &= k_0(u_{2n} + u_{2n+2} - 2u_{2n+1}) \\ M_2 \frac{d^2}{dt^2} u_{2n} &= k_0(u_{2n-1} + u_{2n+1} - 2u_{2n}) \end{aligned}\right\} \quad (6)$$

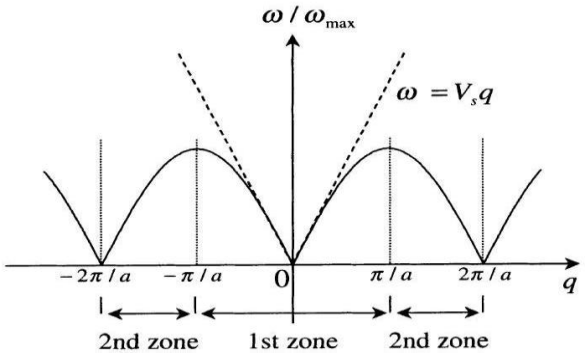

Fig. 2. Dispersion curve of one-dimensional lattice vibration for the atoms M_1 and M_2. We assume once again wave-type solutions of the same type as before. In addition we may expect another type of solution where atoms of even order and odd order are displaced in the reverse direction to each other, and thus atoms of even

order form a wave and odd order atoms form another wave. To satisfy these vibration types we express the displacement as

$$u_{2n+1} = A_1 e^{i\{(2n+1)(qa/2)-\omega t\}},\ u_{2n} = A_2 e^{i\{(2n)(qa/2)-\omega t\}} \quad (7)$$

Inserting these equations into (6), we obtain following relations:

$$\left.\begin{aligned}(M_1\omega^2 - 2k_0)A_1 + \{2k_0\cos(qa/2)\}A_2 = 0\\ (M_2\omega^2 - 2k_0)A_2 + \{2k_0\cos(qa/2)\}A_1 = 0\end{aligned}\right\} \quad (8)$$

We easily find that the condition $A_1 = A_2 = 0$ correspond to all atoms at a standstill, and therefore we have to find solutions such that both A_1 and A_2 are not zero simultaneously. This condition is satisfied by requiring the determinant of the simultaneous equations with respect to A_1 and A_2 in (8) to be zero, giving rise to

$$\begin{vmatrix}(M_1\omega^2 - 2k_0) & 2k_0\cos(qa/2)\\ 2k_0\cos(qa/2) & (M_2\omega^2 - 2k_0)\end{vmatrix} = 0. \quad (9)$$

This equation is regarded as a quadratic equation with respect to ω^2, and the solutions ω_-^2 and ω_+^2 are given by

$$\omega_-^2 = \frac{-k_0}{M_1M_2}\left[(M_1+M_2) - \sqrt{(M_1+M_2)^2 - 4M_1M_2\sin^2\left(\frac{qa}{2}\right)}\right], \quad (10a)$$

$$\omega_+^2 = \frac{k_0}{M_1M_2}\left[(M_1+M_2) - \sqrt{(M_1+M_2)^2 - 4M_1M_2\sin^2\left(\frac{qa}{2}\right)}\right]. \quad (10b)$$

It is evident from (10b) and (10b) that $\omega_-$and ω_+approach zero and a constant not equal to zero as $q \to 0$. Taking account of the fact that the

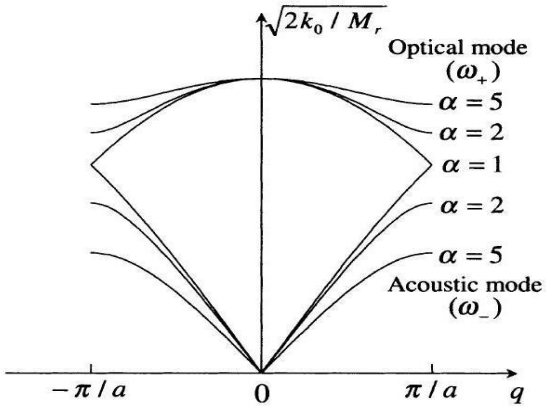

Fig. 3. Angular frequency versus wave vector relations for the two vibration modes of a lattice consisting of two kinds of atoms angular frequency is positive, ω_- and ω_+ are plotted as a function of the wave vector q for several values of $\alpha = M_1/M_2$ as a parameter in Fig. 3, where we define $1/M_r = 1/M_1 + 1/M_2$. Let us consider the two branches ω_- and ω_+ inthe long wavelength limit. For $q = 0, (8), (10\ b)$ and (10b) lead us to the following results:

$$\left.\begin{aligned} &\omega_- = 0 \\ &\frac{A_1}{A_2} = 1 \end{aligned}\right\}$$
$$\left.\begin{aligned} &\omega_+ = \sqrt{2k_0\left(\frac{1}{M_1}+\frac{1}{M_2}\right)} \equiv \sqrt{\frac{2k_0}{M_r}} \\ &\frac{A_1}{A_2} = -\frac{M_2}{M_1} \end{aligned}\right\} \quad (12)$$

RESULTS

When we put $M_1 = M_2$, the ω_- branch gives the same result as a lattice consisting of one kind of atom, corresponding to a sound wave, and thus called the acoustic branch, the acoustic mode of vibrations or the acoustic phonon. Since the acoustic branch satisfies the condition $(A_1 = A_2)$, the neighboring atoms move in the same direction and thus the relative displacement is zero in the long wavelength limit. On the other hand, the ω_+ branch satisfies $A_1/A_2 = -M_2/M_1$ and thus different atoms are displaced in the opposite directions to each other, resulting in zero of the center of mass motion. The ω_+ branch exhibits a relative displacement between the different atoms and induces an electric field when the atoms are ionic. The induced electric field interacts strongly with the external electromagnetic field and absorbs the external waves. This often occurs in the infrared region, leading to it to be called the optical branch, optical mode of lattice vibrations or the optical phonon. Figure 6.4 shows a schematic illustration of the atomic displacement for (a) the acoustic mode (acoustic phonon) and (b) the optical mode (optical phonon), where we see the difference in the displacement between the two modes of lattice vibrations.

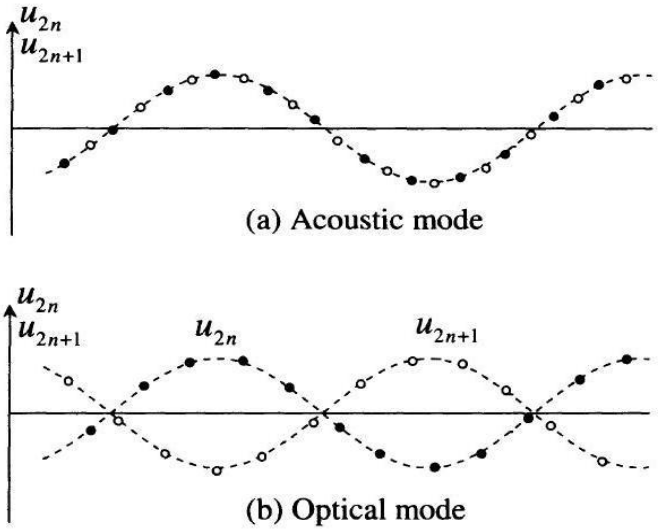

Fig. 4. Schematic illustration of two types of lattice vibrations: (a) acoustic mode (acoustic phonon) and (b) optical mode (optical phonon)

The acoustic mode in the limit of $qa \ll 1$ gives the following relation:

$$\omega_- \cong \sqrt{\frac{2k_0}{(M_1+M_2)}}aq \ (qa \ll 1) \tag{13}$$

and thus the sound velocity (phase velocity) is given by

$$v_s = \frac{\omega_-}{q} = \sqrt{\frac{2k_0}{(M_1+M_2)}}a \tag{14}$$

which corresponds to (5).

DISCUSSION

In ionic crystals unusual reflectivity has been observed in the infrared wavelength region of $20-100\mu$m. For example, the reflectivity of NaCl exhibits maxima around 40μm and 60μm, where the angular frequencies of light for the corresponding wavelengths are $\omega = 2\pi c/\lambda \sim 4\times 10^{13}\ \mathrm{s}^{-1}$ and their wave vectors are $q = 2\pi/\lambda \sim 10^3\ \mathrm{cm}^{-1}$, which are much smaller than the wave vector at the Brillouin zone edge $\pi/a \simeq 10^8\ \mathrm{cm}^{-1}$. From the energy and momentum conservation rules, such high energy excitation in the small wave vector region is easily found to correspond to the optical phonon branch ω_+.

In general, as stated previously, the optical mode of lattice vibration appears in a crystal with two or more atoms in a unit cell. Since there exist one longitudinal and two transverse acoustic modes, a crystal with s atoms in a unit cell gives rise to $3(s-1)$ optical modes of lattice vibration.

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