

Dynamics of a Perturbed Linear Chain of Atoms

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Abstract

Since approximately 1950 an increasing portion of experimental solid state physics research has been concerned with studying defects in crystals. This work uses the code BORN written by Silsbee and Drager to simulate the dynamics of a perturbed linear chain of atoms. Specifically, the dispersion curves for pure and impure monatomic crystal has been obtain. Also the power law dependence of the impurity mode investigated. It has been found that the impurity atom does not alter the shape of the dispersion curve. The effect of the impurity occurs at higher wave vectors, that is, in the lower wavelength limit. As the ratio of the atomic mass of the impurity to the host mass decreases, the maximum angular frequency increases. Also, the power law dependence has been confirmed.

Keywords: Lattice vibration, Dispersion relation, Impurity mode, Defect

1.0 Introduction

It has been observed [1] that since approximately 1950 an increasing portion of experimental solid state physics research has been concerned with studying defects in crystals. However, the theoretical understanding and controlled preparation of compound with defects or random structure has been very slow in developing. This work is intended to contribute positively in our understanding of lattice vibration associated with defects. It is the first part of our intention to investigate the effects of defects in nanotubes.

In this work, a code known as *born*, written by Silsbee and Drager[2], was employed to simulate the dynamics of a perturbed linear chain of atoms. Specifically, the frequencies of the localized modes were computed and the power law dependence of the frequency of the local mode with the mass of the impurity investigated. Also, dispersion curves for pure and impure monatomic crystal were generated and examined.

2.0 Theory

2.1 Normal Modes of Monatomic Linear Chain of Atoms

The atoms of a solid take part in thermal vibrations about their equilibrium positions. Because of a strong interaction between them, the nature of these vibrations turns out to be extremely complex and an accurate description of it present enormous difficulties. Therefore, approximate methods and various simplifications are use to solve this problem.

Instead of describing the individual vibrations of the particles the practice is to consider their collective motion in crystal which is spatially ordered structure. This is based on the fact that powerful bonds immediately transmit the vibrations of one particle to other particles and a collective motion in the form of an elastic wave involving all the particles of the crystals is excited in it. Such collective motion is called the normal mode of a lattice [3]. The number of normal modes coincides with the number of degrees of freedom, which is $3N$ if N is the number of particles constituting the crystal.

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Fig.1 represents a linear chain of atoms separated by a distance a and able to vibrate in the direction perpendicular to the chain. Such a chain may be regarded as a string. If the ends of the chain are fixed, the fundamental mode corresponding to the lowest frequency ω_{\min} is represented by the standing wave with a node at each end. The length of the shortest wave in such a chain is evidently equal to twice the distance between the atoms of the chain (Fig. 2.):

$$\lambda_{\min} = 2a. \tag{1}$$

The corresponding maximum frequency, ω_{\max} is

$$\omega_{\max} = 2\pi v / \lambda_{\min} = \pi v / a, \tag{2}$$

where v is the velocity of wave propagation (of sound) along the chain.

This maximum frequency is a parameter of the chain's material and is determined by the inter-atomic distance and the velocity of wave propagation[4]. Should we set $a = 3.6 \times 10^{-10}m$ (the lattice parameter of copper) and $v = 3550m/s$ (the velocity of sound in copper) we would obtain $\omega_{\max} \approx 3 \times 10^{13} s^{-1}$, which corresponds to the frequency of atomic vibrations in sound.

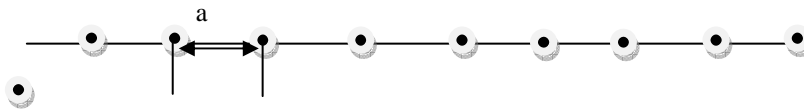


Fig. 1 Normal modes of a linear chain made up of identical atoms.

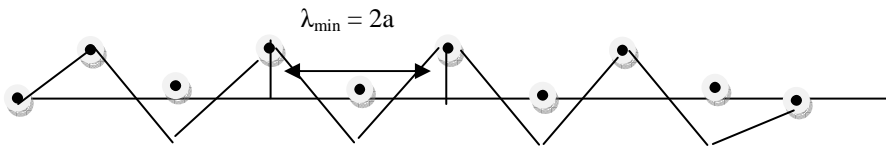


Fig. 2 Normal modes of the chain corresponding to shortest wavelength.

Consider a linear chain of atoms with mass m , separated by lattice constant a , and with only nearest – neighbour interactions. The mass displacements for normal modes have the form $U_s = ue^{i(ksa - wt)}$, and the periodic boundary condition can be written, $e^{ikna} = 1$. The possible values for the scattering wave vector k are then, $k = (2\pi n) / Na$, where n is an integer. Thus, the Newton equation of motion is:[5]

$$m \frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s), \tag{3}$$

where C is the force constant. The above equation can be written as:

$$-m\omega^2 = C(e^{iKa} + e^{-iKa} - 2) \tag{4}$$

so that,

$$\omega^2 = (4C/M) \text{Sin}^2 \frac{1}{2}Ka \tag{5}$$

A complete set of normal modes can be enumerated by solving equation (5) for the values of k within the first Brillion zone[6]. All normal modes solutions to equation (5) are doubly degenerate in frequency with $\omega(k) = \omega(-k)$ except for $k = 0$ and $k = \pi/a$. The dispersion relation $\omega(k)$ is shown in fig. 3.

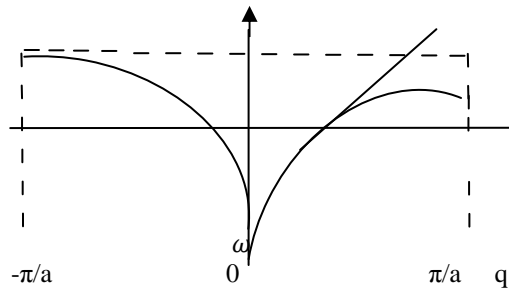


Fig.3. Dispersion Curves of a monatomic linear chain.

To describe wave processes one usually uses the wave vector q whose direction coincides with that of wave propagation and whose absolute value is:

$$q = 2\pi / \lambda \tag{6}$$

It follows from (2) that $2\pi / \lambda = \omega / v$. Therefore,

$$q = \omega / v, \tag{7}$$

The phase velocity V , which enters equation (7) is itself a function of the wave vector q and for a linear chain of atoms bonded by elastic forces is expressed by the following relation [4]:

$$V = V_0 \frac{\sin(\frac{qa}{2})}{\frac{qa}{2}}$$

where V_0 is the velocity of wave propagation in a continuous string. It follows from (8) that for a constant a the velocity v is practically independent of q and is approximately V_0 only in the range of small q 's, where $[\text{Sin}(qa/2)]/qa/2 \approx 1$. In this range ω increases approximately in proportion to q (Fig 4.). As q increases the value of $[\text{Sin}(qa/2)]/(qa/2)$ steadily diminishes. This causes the dispersion curve $\omega(q)$ to flatten out, so that at $q = \pi/a$ it runs parallel to q .

2.2 Localized Mode

The presence of light mass impurities in addition to scattering the lattice waves of the host crystal, can give rise to localized modes. These are normal modes of motion of the crystal which decay exponentially with distance from the impurity instead of extending throughout the crystal [2].

For $m < M$, a new mode with frequency above the highest mode appears when the linear chain is localized spatially. Its eigenvector shows the impurity moving with large amplitude, the neighbours of the impurity moving with considerably less amplitude etc. Thus the eigenvector does not have simple harmonic spatial dependence. The presence of the one impurity (M at m) leaves only a single reflection plane at m so that there must be even and odd (symmetric and antisymmetric) solutions[6]

3.0 The Born Code

Born is a lattice dynamics simulation of a one –dimensional chain of atoms. The simulated crystal can be pure or have a mass defect, and the nearest neighbour potential can be purely harmonic or contain an additional quartic component. (Silsbee and Dragger, 1997). *Born* reveals many features of the atomic motion in crystals. Most importantly it can be used to find the normal modes of a periodic array of a very large number of atoms. The code has nine build-in presets and a user can also set up a project. The code has five main menus namely: quit, display, configure, presets and help. These are located at the top of the main window. For each preset the result of the simulation is shown in two displays. At the top there is a graphical display showing the oscillations of the atoms and the propagation of the wave

through the chain. Also, there is at the bottom-right corner a display of variation of the displacement with time for an atom. In addition to the menus, there are additional dialog boxes which are displayed at the bottom-left corner of the main window. These dialogs are: run, initialize, boundary conditions, initials, crystal-type and speed. Also, there are other dialog boxes depending on the choice of the presets. These include amplitude, wave vector, packet width, peak position, impurity mass, and speed. For each of the presets there are additional common menus which are displayed at the bottom-left corner of the main window. These menus are: run, initialize, boundary conditions, initials, crystal-type and speed. In addition there are other menus depending on the choice of the presets. These include amplitude, wave vector, packet width, peak position, impurity mass, and speed.

4.0 Result and Discussion

4.1 Dispersion Relation

The graph of angular frequency versus scattering wave vector (k) (dispersion curve) for the monatomic linear chain is shown in fig. 4. This curve shows the reduced representations for a one – dimensional monatomic lattice with a lattice constant a . It is also the so – called acoustical longitudinal branch of the vibrational spectrum. This vibrational frequencies are of the order of the frequencies of sound waves in the crystal[7].

It has been found that the impurity atom does not alter the shape of the dispersion curve, that is, it rises steadily and flattens as k tends to 1.0. The effect of the impurity occurs at higher scattering wave vectors, that is, in the lower wavelength limit. As the ratio of the atomic mass of the impurity to the host mass (m^*/m) decreases (i.e as we deviate from the pure chain) the maximum angular frequency, ω_{max} increases. Similar result has been observed by Kaplan[8] for the special case of impurity layer on surface waves.

The observed shape of the dispersion curve can be explained as follows. It follows from eqn. (8) that for a given lattice constant a the velocity v is practically independent of q and is approximately V_0 only in the range of small q 's, where $[\text{Sin}(qa/2)]/qa/2 \approx 1$. In this range ω increases approximately in proportion to q . As q increases the value of $[\text{Sin}(qa/2)]/(qa/2)$ steadily diminishes. This causes the dispersion curve $\omega(q)$ to flatten out, so that at $q = \pi/a$ it runs parallel to q .

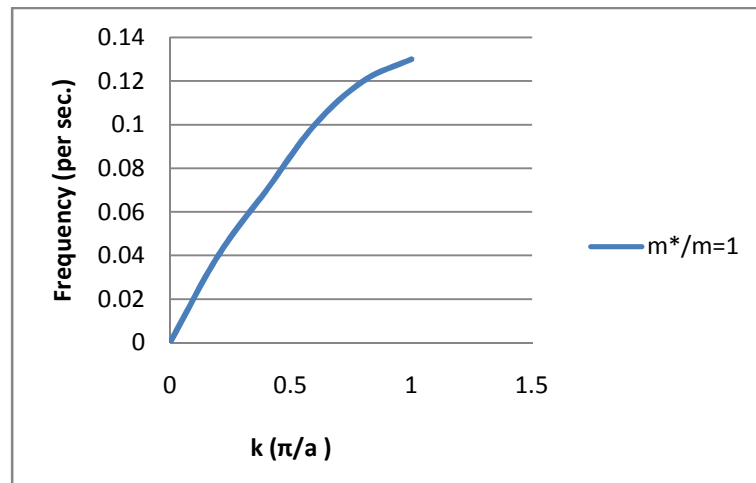


Figure 4(a) Dispersion curve for pure monatomic crystal

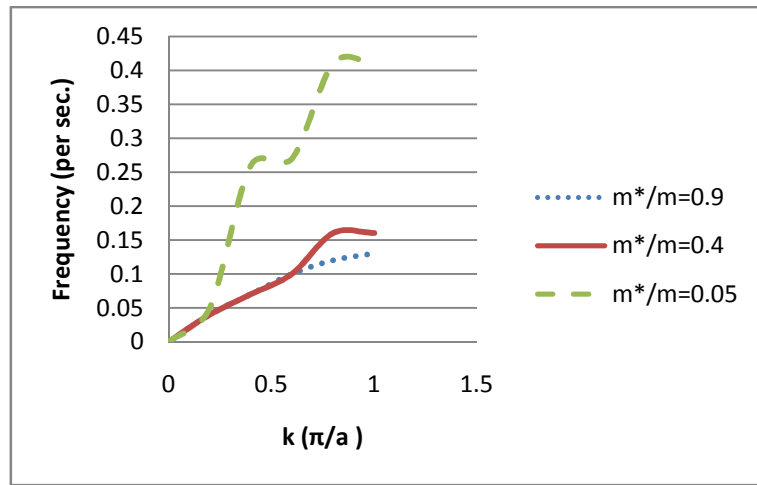


Figure 4(b) Dispersion curves for Impure monatomic crystal

4.2 Power law Dependence of the Impurity mode

From equation (5) the maximum angular frequency, $\omega_{max}^2 = 4C/M$ i.e $\omega_{max} = 2\sqrt{C/M}$. For a continuum chain, C is simply the spring constant. The power law dependence of the impurity mode i.e graph of $\log T$ against $\log m^*/m$, where T is the period of the localized mode, is shown in fig. 5. It can be seen that a straight line is obtained, suggesting that, $\log T$ and $\log m^*/m$ obey the power law relationship[9]. Hence, the power law dependence has been confirmed.

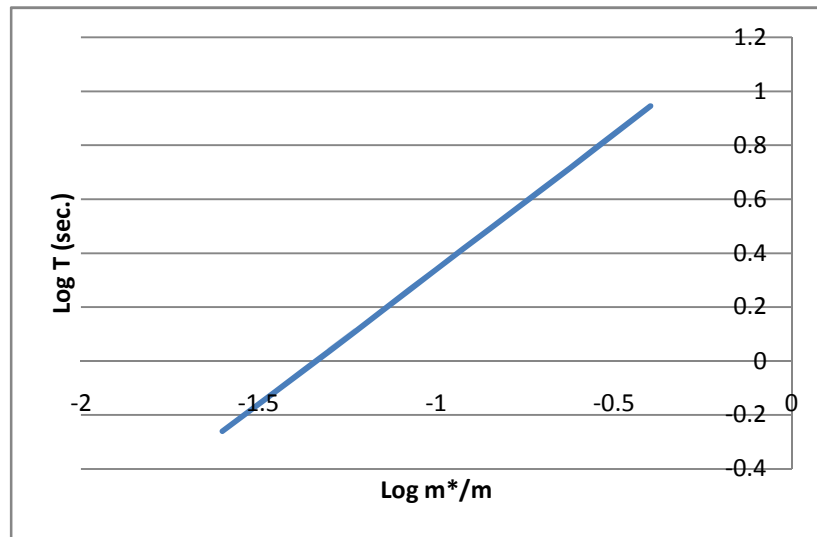


Figure 5: graph of log T against log m*/m.

4.3 Effects of Boundary Conditions in the Born Simulation Code

The program employs two types of boundary conditions, namely periodic boundary condition and fixed boundary condition.

The observed effects of the periodic boundary conditions are:

- All the atoms vibrate about their mean positions.
- The displacements of the atoms could be large enough to the extent that they diffuse out of their original cells.
- The atomic displacements depends on the wave vector and that, it decreases on increasing wave vector.

Journal of the Nigerian Association of Mathematical Physics Volume 20 (March, 2012), 267 – 272

However, the effects observed in the case of fixed boundary conditions are:

- The atoms at the end of the chain are static, but other atoms vibrate about their mean positions.
- The displacements of the atoms is independent of the wave vector.
- The vibration of an atom is confined to the region of the cell (*i.e.* the atoms do not diffuse out of their own cells).

5.0 Summary and Conclusion

The code *born* has been used to simulate the dynamics of a perturbed linear chain of atoms. The perturbed chain consist of atoms of mass m with one of them replaced by an atom of mass M . The dispersion curve for the pure linear chain has been obtained and agree with the exact result. The impurity atom does not change the shape of the dispersion curve, however, as the ratio (m^*/m) decreases, the maximum angular frequency, ω_{max} of the perturbed chain increases above that of the pure chain. Finally, the power law dependence has been confirmed.

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