------ Raf. Jour. Sci., Vol. 16, No. 1 Physics, Special Issue, pp. 89-94, 2005 ------

Theoretical Study of Longitudinal Vibrations of Two Coupled Crystal Slabs Using Difference Equations Method

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(Received 9/12/2003 ; Accepted 28/11/2004)

ABSTRACT

A Mathematical model describing lattice vibration is built for solid state lattice. The lattice considered consist of two crystal slabs with different atoms. Difference equation method formed the building stone of the model. Results of calculation indicate good agreement with results obtained by other authors.

دراسة نظرية للاهتزازات الطولية لشريحتين بلوريتين مرتبطتين مع بعضهما باستخدام معادلات الفرق

الملخص

تم بناء نموذج رياضي لوصف الاهتزازات الشبيكية لشبيكة صلبة. تم اختيار شبيكة تتكون من شريحتين من ذرات مختلفة واستندت الدراسة على استخدام معادلات الفرق في بناء النموذج الرياضي. أظهرت الحسابات وجود اتفاق جيد مع نتائج البحوث الأخرى لهذا النوع من الشبيكة.

INTRODUCTION

A crystal may be viewed as large number of point atoms which are arranged in space in a regular lattice sites by small distances impaled by harmonic forces of interaction with their neighbors (Rosenstock,1955;Ghatak and Kothari,1972;Patterson, 1971). Study of atomic and lattice vibration in a particular crystal can lead to useful information concerning many physical phenomena. Such phenomena include spin-lattice relaxation, neutron scattering, … etc.

As an example for crystal lattice, many authers studied a one-dimensional linear atomic chains (Wallis, 1956; Gazis and Wallis, 1962; Grosse et al., 1981; Mossa, 2003).

The vibrational problem of slab-shape diatomic ionic crystal is studied in the harmonic approximation and retardation effect by (Fuchs and Kliewer, 1965; Kliewer and Fuchs, 1966; Lucas, 1968; Grosse et al., 1981). Lucas used Kellermann's model, which consist of point-charge ions interacting through a nearest neighbor repulsive forces and long-range dipole-dipole forces.

In the present work we consider a model similar to Lucas model of two crystal slabs, which consist of two double linear chains coupled together as shown in (fig.1). we assume that the particles are held together by elastic forces obeying Hook's law, and these particles execute longtudinal vibrations only.

In the present work we neglected the attraction force between the upper and lower atoms in the slabs, because we interested in the longitudinal vibrations only, and we considered the two slabs so thin as possible because each slab consists of two long linear chains,and the correction made by τ and τ_2 is very small, and not make a larger difference in the coupling constants.

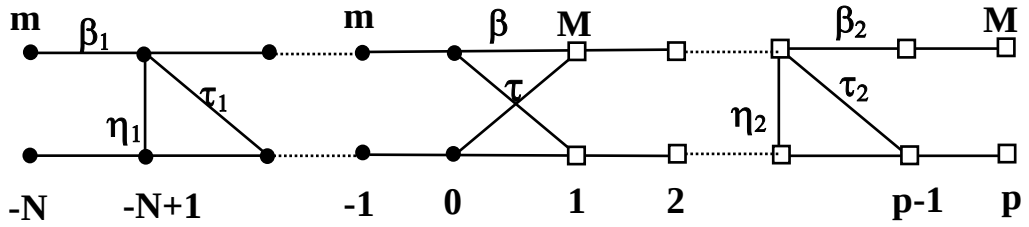

Fig.1: A Model of two Crystal Slabs coupled through nearest neighbor forces.

The first double chain consist of identical particles of mass m, lying in the lattice points from (-N to 0) lattice point. The second double chain consist of identical particles of mass M, (m ≠M), lying in the lattice points 1 to p.

For the coupling constants see (fig.1)

β_1, η_1, τ_1 are the force constants for the first double chain.

β_2, η_2, τ_2 are the force constants for the second double chain.

β, τ are the force constants between the two double chains.

Equations of Motion for Lattice Vibrations and their Solutions:

As the system considered is of two coupled double chains, one needs to evaluate a two dimensional lattice. We may choose the 0 number lattice point as an origin, the points on the right of it are numbered 1, 2, …,p and those on the left are numbered –1, -2, …, -N. As we are limited with nearest neighbor interaction, then the displacement of the nth particle from its equilibrium position will be denoted by U_n. Since we have assumed that the forces between particles obeys Hookes law, the energy of interaction between any two particles will be a function of the displacement between them only. So the equation of motion of these particles at any time build a system of (p+N+1) homogenous differential equations (Mossa, 2003).

1. For lattice point n = -N, we obtain:

$$m\ddot{U}_{-N} = -\beta_1\left(U_{-N} - U_{-N+1}\right) - \tau_1\left(U_{-N} - U_{-N+1}\right) \quad (1)$$

for the time dependence of U_n we use the factor exp(-iωt) (Patterson, 1971; Mossa, 2003). Then we can write the time independent difference equation for (1) as follows

$$(m\omega^2 - \gamma)\, U_{-N} + \gamma\, U_{-N+1} = 0 \quad (2)$$

where $\gamma = \beta_1 + \tau_1$ (which is a constant)

2. For the lattice points $-N+1 \le n \le -1$, we obtain:

$$m\ddot{U}_n = -\beta_1(2U_n - U_{n+1} - U_{n-1}) - \tau_1(2U_n - U_{n+1} - U_{n-1}) \quad (3)$$

Then the time independent equation for (3) is as follows

$$U_{n+1} + \left(\frac{m\omega^2}{\gamma} - 2\right)U_n + U_{n-1} = 0 \quad (4)$$

Equation (4) is second order difference equation. Using the general theory of difference equations (Valenta and Jager, 1977; Valenta and Jager, 1981, Gasagronde, 1981; Jager et al., 1988; Mossa, 2003) with $U_n = \lambda^n$. We can write the characteristic equation for equation (4) in the following form

$$\lambda^{n+1} + \left(\frac{4\omega^2}{\omega_{max}^2} - 2\right)\lambda^n + \lambda^{n-1} = 0 \quad (5)$$

where

$$\omega_{max}^2 = \frac{4\gamma}{m}$$

Then, after dividing by λ^{n-1}, we obtain

$$\lambda^2 + \left(\frac{4\omega^2}{\omega_{max}^2} - 2\right)\lambda + 1 = 0 \quad (6)$$

which has the following solutions

$$\lambda_{1/2} = \left(1 - \frac{2\omega^2}{\omega_{max}^2}\right) \mp \frac{2\omega}{\omega_{max}^2}\sqrt{\omega^2 - \omega_{max}^2} \quad (7)$$

These solutions are complex conjugate and the general solution for difference equations (4) is given by

$$U_n = c_1 e^{i\varphi n} + c_2 e^{-i\varphi n} \quad (8)$$

c_1 and c_2 are constants

where

$$\tan\varphi = \frac{\left(\frac{4\omega^2}{\omega_{max}^2} - \frac{4\omega^4}{\omega_{max}^4}\right)^{1/2}}{\left(1 - \frac{2\omega^2}{\omega_{max}^2}\right)} \quad (9)$$

3. For the origin lattice point $n = 0$, we have

$$m\ddot{U}_o = -\beta_1(U_o - U_{-1}) - \beta(U_o - U_1) - \tau_1(U_o - U_{-1}) - \tau(U_o - U_1) \quad (10)$$

The time independent equation for equation for (10) is giving by

$$(m\omega^2 - \gamma - \alpha)U_o + \gamma U_{-1} + \alpha U_1 = 0 \quad (11)$$

where $\alpha = \beta + \tau$ (which is a constant)

4. For the point $n = 1$, we obtain

$$m\ddot{U}_1 = -\beta(U_1 - U_o) - \beta_2(U_1 - U_2) - \tau(U_1 - U_o) - \tau_2(U_1 - U_2) \quad (12)$$

And its time independent equation is of the form

$$(M\omega^2 - \mu - \alpha)U_1 + \mu U_2 + \alpha U_o = 0 \quad (13)$$

Where $\mu = \beta_2 + \tau_2$ (which is a constant)

5. For lattice points $2 \le n \le p\text{-}1$, we obtain

$$M\ddot{U}_n = -\beta_2(2U_n - U_{n-1} - U_{n+1}) - \tau_2(2U_n - U_{n-1} - U_{n+1}) \quad (14)$$

And the time independent equation for (14), has the following form

$$U_{n+1} + \left(\frac{M\omega^2}{\mu} - 2\right)U_n + U_{n-1} = 0 \quad (15)$$

Which is a second order difference equation, and after using general theory of difference equations (Valenta and Jager, 1977; Valenta and Jager, 1981; Jager et al., 1988), we find that

$$\lambda^{n+1} + \left(\frac{4\omega^2}{\overline{\omega}^2_{max}} - 2\right)\lambda^n + \lambda^{n-1} = 0 \quad (16)$$

Where $\overline{\omega}^2_{max} = \dfrac{4\mu}{M}$

Then, after dividing by λ^{n-1}, we obtain

$$\lambda^2 + \left(\frac{4\omega^2}{\overline{\omega}^2_{max}} - 2\right)\lambda + 1 = 0 \quad (17)$$

Which has the following solutions

$$\lambda_{1/2} = \left(1 - \frac{2\omega^2}{\overline{\omega}^2_{max}}\right) \mp \frac{2\omega}{\overline{\omega}^2_{max}}\sqrt{\omega^2 - \overline{\omega}^2_{max}} \quad (18)$$

Which are complex conjugate solutions

Then, the general solution of the difference equation (15) has the following form

$$U_n = c_1^1 e^{i\theta n} + c_2^1 e^{-i\theta n} \quad (19)$$

Where c_1^1, c_2^1 are constants, and

$$\tan\theta = \frac{\left(\dfrac{4\omega^2}{\overline{\omega}^2_{max}} - \dfrac{4\omega^4}{\overline{\omega}^4_{max}}\right)^{1/2}}{\left(1 - \dfrac{2\omega^2}{\overline{\omega}^2_{max}}\right)} \quad (20)$$

6. For the lattice point $n = p$, we obtain

$$M\ddot{U}_p = -\beta_2(U_p - U_{p-1}) - \tau_2(U_p - U_{p-1}) \quad (21)$$

And its time independent difference equation is of the form

$$(M\omega^2 - \mu)\, U_p + \mu\, U_{p-1} = 0 \quad (22)$$

When we substitute the general solution for the first crystal slab from equation (8) into the boundary lattice point –N and its nearest neighbor (-N+1), we obtain the relation:

$$c_2 = c_1 e^{-i\varphi(2N+1)} \tag{23}$$

Similarly, after substituting the general solution for the second crystal slab from equation (19) into the another boundary lattice point p and its nearest neighbor (p-1) , we obtain the relation

$$c_2^1 = c_1^1 e^{i\theta(2p+1)} \tag{24}$$

Using the general solutions from equations (8) and (19), we can write

$$\left.\begin{aligned} U_o &= c_1 e^{i\varphi(o)} + c_2 e^{-i\varphi(o)} \\ U_{-1} &= c_1 e^{-i\varphi} + c_2 e^{i\varphi} \\ U_1 &= c_1^1 e^{i\theta} + c_2^1 e^{-i\theta} \\ U_2 &= c_1^1 e^{i2\theta} + c_2^1 e^{-i2\theta} \end{aligned}\right\} \tag{25}$$

When we substitute equations (25) into equation (11) and making use of equations (23) and (24), we obtain

$$\begin{aligned} &c_1\left[\left\{\left(m\omega^2 - \gamma - \alpha\right) + \gamma e^{-i\varphi}\right\} + \left\{\left(m\omega^2 - \gamma - \alpha\right) + \gamma e^{i\varphi}\right\} e^{-i\varphi(2N+1)}\right] \\ &\quad + c_1^1\left[\alpha e^{i\theta} + \alpha e^{-i\theta} + e^{i\theta(2p+1)}\right] = 0 \end{aligned} \tag{26}$$

Know when we substitute equations (25) into equation (13) and making use of equations (23) and (24), we obtain

$$\begin{aligned} &c_1^1\left[\left\{\left(M\omega^2 - \mu - \alpha\right) e^{i\theta} - \mu e^{-2i\theta}\right\} + \left\{\left(M\omega^2 - \mu - \alpha\right) e^{-i\theta} + \mu e^{-i2\theta}\right\} e^{i\theta(2p+1)}\right] \\ &\quad + c_1\left[\alpha + \alpha e^{-i\varphi(2N+1)}\right] = 0 \end{aligned} \tag{27}$$

When we solve equations (26) and (27) together, then we obtain the general equation of motion for the coupled crystal slabs in the following form

$$\begin{aligned} &2\sin\frac{\varphi}{2}\sin\varphi\left(N+1\right)\sin\frac{\theta}{2}\sin\theta p - \frac{\alpha}{\gamma}\sin\frac{\theta}{2}\sin\theta p\cos\varphi(N+\frac{1}{2}) \\ &\quad - \frac{\alpha}{\mu}\sin\frac{\varphi}{2}\sin\varphi(N+1)\cos\theta(p-\frac{1}{2}) = 0 \end{aligned} \tag{28}$$

Relation (28) is a general equation of vibration for longtudinal vibrations of two coupled crystal slabs with different atoms and different coupling constants, coupled together and forming a system of two-dimensional crystal slabs, and is valid for any atom in the slab.

Special Cases:

1. When $\beta = 0$, $\tau = 0$ i.e. $\alpha = 0$

This Means that we have uncoupled two slab-shape chains with one another, after substituting in equation (28) we obtain:

$$\sin\frac{\varphi}{2}\sin\varphi\,(N+1) = 0 \tag{29}$$

and

$$\sin\frac{\theta}{2}\sin\theta\, p = 0 \tag{30}$$

Which is in full agreement with (Mossa, 2003).

2. When m = M, this means $\beta = \beta_1 = \beta_2$, $\tau = \tau_1 = \tau_2$ and $\alpha = م = ى$.

This leads to a slab-shape atomic chain consisting of identical atoms and identical coupling constants.

Substituting all these in equation (28) and using p = N + 1, we obtain:

$$2\cos\theta\,(N+1) = 0 \tag{31}$$

and

$$\sin\frac{\theta}{2}\sin\theta\,(N+1) = 0 \tag{32}$$

Equations (31) and (32) shows full agreement with (Gasagraude,1981;Jager, 1988).

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