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NUMERICAL SOLUTION OF THE INTERRELATED DIFFERENTIAL EQUATION OF MOTION IN PHONON ENGINEERING

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Abstract. In this work, we study numeric calculations of phonon modes in nanostructures. The motion equation of atoms in a crystal with some simplification, results in a second order ordinary differential equation and two interrelated second order differential equations for 3 polarizations according to 3 dimensions. Although first equation can easily be solved, the next two interrelated equations cannot be solved by usual numerical methods. Based on discretization, a new technique is proposed for studying the motion equations. The results are presented by dispersion curves for shear, dilatational, and flexural modes of phonons.

Keywords: Numeric approximation, Eigenvalue problem, Dispersion curve.

AMS Subject Classification: 65f15, 65L12, 65L16.

1. Introduction

In physics and electronics, the quantized energies of elastic vibration in a crystal are called phonons. Similar to electrons, phonons are characterized by their dispersion $\omega(q)$, where ω is an angular frequency, and q is three dimensional wave vector of a phonon [1]. In order to find the phonon dispersion, the equation of motion for elastic vibration should be solved. In general, the equation of motion for the elastic vibrations in an anisotropic medium can be written as [2,3]

$$\rho\frac{\partial^2 U_m}{\partial t^2} = \frac{\partial \sigma_{mi}}{\partial x_i} \qquad m, i = x, y, z \tag{1}$$

where $\vec{U}\,(U_x, U_y, U_z)$ is the displacement vector in three dimensions, ρ is the mass density of the materials, σ_{mi} is the elastic stress tensor and is equal to $\sigma_{mi} = C_{mikj}S_{kj}$; with S_{kj} being the strain tensor, C_{mikj} being the fourth-order tensor and *i, j,* and k are three *x,y,z* directions. Because of symmetry in the above equations S_{kj} and σ_{mi}, as shown in equations (2) and (3), the 3×3 matrices of stress and strain diminishes to six element vectors.

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Furthermore, the forth order tensor of stiffens factors, C_{mikj}, converts to a symmetric two-index notation presented with C_{ij}.

$$S_{kj} = \begin{bmatrix} S_{xx} & S_{xy} & S_{xz} \\ S_{yx} & S_{yy} & S_{yz} \\ S_{zx} & S_{zy} & S_{zz} \end{bmatrix}, \qquad S_{xy} = S_{yx}\ , \qquad S_{xz} = S_{zx}, \qquad S_{yz} = S_{zy}, \tag{2}$$

$$\sigma_{mi} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix}, \qquad \sigma_{xy} = \sigma_{yx}\ , \qquad \sigma_{xz} = \sigma_{zx}, \qquad \sigma_{yz} = \sigma_{zy}. \tag{3}$$

Adopting the two-index notation as: $xxxx \to 11$; $yyyy \to 22$; $zzzz \to 33$; $xxyy \to 12$; $xxzz \to 13$; $yzyz \to 44$; $xzxz \to 55$; $xyxy \to 66$, leads to [4,5]:

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & SYM & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{bmatrix} \begin{bmatrix} S_{xx} \\ S_{yy} \\ S_{zz} \\ S_{yz} \\ S_{xz} \\ S_{xy} \end{bmatrix}. \tag{4}$$

In this research we consider the wurtzite crystals for layers for which the 6×6 matrix of the elastic constants C_{ij} is given in [6]:

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}. \tag{5}$$

The axis x is assumed to be along the propagation direction of the waves. Since the considered structure is a multi-layer hetero-structure with layer growth direction along the z-axis (non-uniform along the z-axis), ρ and C_{ij} $(i,j=1,\ldots,6)$ depend on the z coordinate only. We look for a numerical solution [7-12] of equation (1) in the following form of sinusoidal traveling waves subjected to appropriate boundary conditions

$$U_i\,(x,z,t) = u_i\,(z)\,e^{i(wt-qx)}, \qquad i = x,y,z. \tag{6}$$

where u_i are the amplitudes of the displacement vector components. Substituting equation (6) for $i = y$ in equation (1), the partial differential equation (1) transforms into an ordinary second order differential equation as below[5]

$$-\rho(z)\omega^2 u_y(z) = C_{44}(z)\cdot\frac{d^2u_y(z)}{dz^2} + \frac{dC_{44}(z)}{dz}\cdot\frac{du_y(z)}{dz} - C_{66}(z)q^2u_y(z), \tag{7}$$

with the initial condition resulting from force equilibrium on the outer surfaces by:

$$\frac{\partial u_y}{\partial z}|_{z=\pm L/2} = 0. \tag{8}$$

Substituting equation (6) for $i = x, z$ in equation (1), the following two interrelated equations results[5]

$$-\rho\omega^2u_x(z) = -q^2C_{11}u_x(z) + C_{44}\frac{d^2u_x(z)}{dz^2} + q(C_{11}+C_{44})\frac{du_z'(z)}{dz} + \frac{dC_{44}}{dz}\left(\frac{du_x(z)}{dz} + qu_z'(z)\right), \tag{9}$$

$$\begin{aligned}-\rho\omega^2 u'_z(z) = &- q^2 C_{44} u'_z(z) + C_{33}\frac{d^2 u'_z(z)}{dz^2} + \frac{dC_{33}}{dz}\frac{du'_z(z)}{dz} \\ &- q\left[(C_{44}+C_{13})\frac{du'_z(z)}{dz} + \frac{dC_{13}}{dz}u_x(z)\right], \qquad (10)\end{aligned}$$

where $u'_z = -iu_z$, and the boundary conditions on the outer surfaces of structure yields:

$$\left.\frac{\partial u_x}{\partial z} + qu'_z\right|_{z=\pm L/2} = 0, \qquad (11)$$

$$\left.C_{33}\,\frac{\partial u'_z}{\partial z} - qC_{13}u_x\right|_{z=\pm L/2} = 0. \qquad (12)$$

2. Results:

By discretization and using finite difference method for solving the equation (7), it could be converted to an eigenvalue problem (EVP). Since the materials are homogenous, derivative$(dC_{44}(z))/dz$ is zero everywhere other than on the boundaries. Even on the boundaries, the derivative is ignored because the C_{44} is very close for the two adjacent layers. The equation (7) converts to the following matrix equation

$$\mathbb{A}u = \omega^2 u, \qquad (13)$$

where A is an $n \times n$ tri-diagonal matrix, u is displacement vector with n points, and is angular frequency corresponding to each wave vector q. The matrix A will be of the form

$$\mathbb{A} = 1/h^2 \begin{bmatrix} A_s & A_1 & & & & & & & \\ A_2 & A_3 & A_1 & & & & & & \\ & A_2 & A_3 & A_1 & & & & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & A_2 & A_3 & A_1 & & & \\ & & & & A_2 & A_3 & A_1 & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & & & & A_2 & A_3 & A_1 \\ & & & & & & & A_2 & A_e \end{bmatrix} \qquad (14)$$

where $A_s = A_e = \frac{{C_{44}}^n - q{C_{66}}^n}{\rho^n}$, $A_1 = \frac{-{C_{44}}^{n+1}}{\rho^{n+1}}$, $A_2 = \frac{-{C_{44}}^{n-1}}{\rho^{n-1}}$, $A_3 = \frac{2{C_{44}}^n - q{C_{66}}^n}{\rho^n}$, h is differential element, and n is row index. For each value of the vector q in $A_{3,s,e}$, one can solve the equation (13) as an eigenvalue problem (EVP). Solving the EVP, the resulted eigenvectors represent the displacement vectorsand the eigenvalues represent square of corresponding angular frequencies. Varying q from its minimum to maximum and solving the associated EVP, the dispersion curves of phonon are found. These modes or polarization of displacement of atoms have been named shear modes. Six smallest shear modes of acoustic phonons for a three layer hetero-structure are shown in Fig.1.

For the other two vibrational polarizations of the displacement vector components u_x and u_z, are obtained by substituting equation (6) in equation (1) (for $i = x, z$). The resulted equations (9) and (10), interrelated and could not be solved easily as equation (7). Taking an equally spaced mesh and using the central difference approximation for $\frac{d^2}{dz^2}$

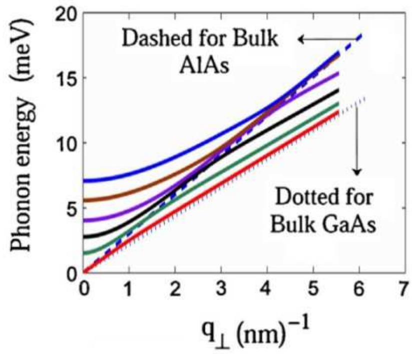

Figure 1. Shear modes for 9129 nm AlAs-GaAs-AlAs heterostructure [1].

with error $O(h^2)$ and forward difference approximation for $\frac{d}{dz}$ in (9) and (10) yields the approximating schemes:

$$\frac{-1}{\rho}C_{44}\frac{1}{h^2}u_x^{i-1}+\left(\frac{2C_{44}}{\rho h^2}+q^2\frac{C_{11}}{\rho}\right)u_x^i-\frac{C_{44}}{\rho h^2}u_z^{i+1}+ \frac{q(C_{13}+C_{44})}{\rho h}u_z^{i-1}+\frac{-q(C_{13}+C_{44})}{\rho h}u_z^i=\omega^2u_x^i, \qquad (15)$$

$$\frac{-1}{\rho h}(C_{13}+C_{44})u_x^{i-1}+\frac{q}{\rho h}\left(C_{13}+C_{44}\right)u_x^i+\frac{-C_{33}}{\rho h^2}u_z^{i-1}+ \left(\frac{2C_{33}}{\rho h^2}+q^2\frac{C_{44}}{\rho}\right)u_z^i-\frac{C_{33}}{\rho h^2}u_z^{i+1}=\omega^2u_z^i. \qquad (16)$$

Now incorporating the boundary conditions, (11) gives

$$u_x^0=u_x^1+hqu_z^1, \qquad (17)$$

$$u_x^{N+1}=u_x^N+hqu_z^N, \qquad (18)$$

for $i=1$ and $i=N$, respectively. Moreover from the boundary condition (12) we get

$$u_z^0=\frac{-hqC_{13}}{C_{33}}-u_z^1, \qquad (19)$$

$$u_z^{N+1}=\frac{-hqC_{13}}{C_{33}}-u_z^N. \qquad (20)$$

Substituting (17) and (19) in the first point of (9) and (10) ($i=1$), one can deduce

$$\left[\frac{C_{44}}{\rho h^2}+q^2\frac{C_{11}}{\rho}-\frac{q^2C_{13}\left(C_{13}+C_{44}\right)}{\rho C_{33}}\right]u_x^1-\frac{C_{44}}{\rho h^2}u_x^2+\left[\frac{-q\left(2C_{13}+3C_{44}\right)}{\rho h}\right]u_z^1=\omega^2u_x^1, (21)$$

$$\frac{-C_{13}q}{\rho h}u_x^1+\left[\frac{3C_{33}}{\rho h^2}+\frac{q^2C_{13}}{\rho}\right]u_z^1-\frac{C_{33}}{\rho h^2}u_z^2=\omega^2u_z^1. \qquad (22)$$

Similarly, for $i=N$ in the last point of (9) and (10) using (18) and (20) the following equations are derived

$$\frac{-C_{44}}{\rho h^2}\omega^2u_x^{N-1}+\left[\frac{C_{44}}{\rho h^2}+\frac{q^2C_{11}}{\rho}\right]u_x^N+\frac{q}{\rho h}\left(C_{13}+C_{44}\right)u_z^{N-1}+\left[\frac{-qC_{13}}{\rho h}\right]u_z^N=\omega^2u_x^N, (23)$$

$$\frac{-q(C_{13}+C_{44})}{\rho h}u_x^{N-1}+\frac{q(2C_{13}+C_{44})}{\rho h}u_x^N-\frac{C_{33}}{\rho h^2}u_z^{N-1}+\left[\frac{C_{33}}{\rho h^2}+\frac{q^2C_{44}}{\rho}\right]u_z^N=\omega^2u_z^N. (24)$$

Therefore (9) and (10) can be written in matrix form as the following order n systems

$$\begin{cases} \mathbb{A}u_x + \mathbb{B}u_z = \omega^2 u_x, \\ \mathbb{C}u_x + \mathbb{D}u_z = \omega^2 u_z. \end{cases} \tag{25}$$

So, we have the new eigenvalue problem of order $2n \times 2n$

$$\begin{bmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{C} & \mathbb{D} \end{bmatrix} \begin{bmatrix} u_x \\ u_z \end{bmatrix} = \omega^2 \begin{bmatrix} u_x \\ u_z \end{bmatrix} \tag{26}$$

where

$$u_x = \begin{bmatrix} u_x^1 \\ u_x^2 \\ \vdots \\ \\ u_x^N \end{bmatrix} u_z = \begin{bmatrix} u_z^1 \\ u_z^2 \\ \vdots \\ \\ u_z^N \end{bmatrix} \mathbb{A} = \begin{bmatrix} A_s & A_1 & & & & & \\ A_2 & A_3 & A_1 & & & & \\ & A_2 & A_3 & A_1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & & & & \\ & & & & A_2 & A_3 & A_1 \\ & & & & & A_2 & A_e \end{bmatrix}$$

$$A_s = \frac{{C_{44}}^1}{\rho^1 h^2} + q^2 \frac{[\,{C_{11}}^1 {C_{33}}^1 - (C_{13})^2 - {C_{13}}^1 {C_{44}}^1]}{\rho^1 {C_{33}}^1}, A_1 = -\frac{{C_{44}}^{n+1}}{\rho^{n+1} h^2}, A_2 = -\frac{{C_{44}}^{n-1}}{\rho^{n-1} h^2},$$

$$A_3 = \frac{2{C_{44}}^n}{\rho^n h^2} + q^2 \frac{{C_{11}}^n}{\rho^n}, A_e = \frac{{C_{44}}^N}{\rho^N h^2} + q^2 \frac{{C_{11}}^N}{\rho^N},$$

and

$$\mathbb{B} = \begin{bmatrix} B_s & & & & & & \\ B_1 & B_2 & & & & & \\ & B_1 & B_2 & & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & & & & \\ & & & & & B_1 & B_2 \\ & & & & & & B_1 \quad B_e \end{bmatrix}$$

$$B_s = -\frac{q(2{C_{13}}^1 + 3{C_{44}}^1)}{\rho^1 h}, B_1 = \frac{q({C_{13}}^{n-1} + {C_{44}}^{n-1})}{\rho^{n-1} h}, B_2 = -\frac{q({C_{13}}^n + {C_{44}}^n)}{\rho^n h}, B_e = -\frac{q{C_{13}}^N}{\rho^N h},$$

also

$$\mathbb{C} = \begin{bmatrix} C_s & & & & & & \\ C_1 & C_2 & & & & & \\ & C_1 & C_2 & & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & & & & \\ & & & & & C_1 & C_2 \\ & & & & & & C_1 \quad C_e \end{bmatrix}$$

$$C_s = -\frac{qC_{13}^1}{\rho^1 h}, C_1 = -\frac{q({C_{13}}^{n-1} + {C_{44}}^{n-1})}{\rho^{n-1} h}, C_2 = \frac{q({C_{13}}^n + {C_{44}}^n)}{\rho^n h}, C_e = \frac{q(2{C_{13}}^N + {C_{44}}^N)}{\rho^N h},$$

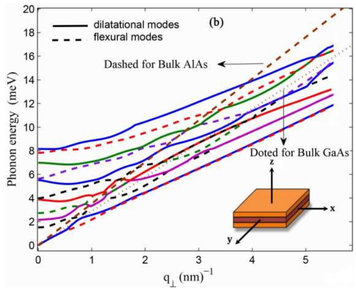

FIGURE 2. Dilatational and flexural modes. $q_\perp$ is in-plane wave vector (q_x, q_y) with 0 to π range.

and finally

$$\mathbb{C} = \begin{bmatrix} D_s & D_1 & & & & & \\ D_2 & D_3 & D_1 & & & & \\ & D_2 & D_3 & D_1 & \ddots & & \\ & & & \ddots & & & \\ & & \ddots & & & & \\ & & & & D_2 & D_3 & D_1 \\ & & & & & D_2 & D_e \end{bmatrix}$$

$$D_s = \frac{3{C_{33}}^1}{\rho^1 h^2} + q^2 \frac{{C_{13}}^1}{\rho^1}, D_1 = -\frac{{C_{33}}^{n+1}}{\rho^{n+1} h^2}, D_2 = -\frac{{C_{33}}^{n-1}}{\rho^{n-1} h^2},$$
$$D_3 = \frac{2{C_{33}}^n}{\rho^n h^2} + q^2 \frac{{C_{44}}^n}{\rho^n}, D_e = \frac{{C_{33}}^N}{\rho^N h^2} + q^2 \frac{{C_{44}}^N}{\rho^N}.$$

For each eigenvalue, ω, there will be u_x and u_z eigenvectors. Because of symmetry in u_x and u_z, we can see that for any ω, when the u_x is symmetrical, the u_z is asymmetrical and vice versa. Due to the spatial symmetry of the considered three layered structure and the mathematical form of Eqs.(9) and (10), the displacement vector should have components with opposite parity, e.g. (u_x^S, u_z^A), when u_x is a symmetrical function of z while u_z is an asymmetrical function of z; or (u_x^A, u_z^S) for the case u_x is an asymmetrical function of z while u_z is a symmetrical function. The (u_x^S, u_z^A) and (u_x^A, u_z^S) have been denoted with u^{SA} and u^{AS} respectively. The upper indices SA and AS of displacement vectors distinguish independent vibrational polarizations which, together with the shear modes, compose a full set of normal vibrational modes in the structure. In the case of a slab the SA modes are referred to as dilatational modes while AS modes are termed the flexural modes. As a result, for the same structures whit shear modes shown in Fig.1, the dilatational and flexural modes of phonon or atom displacements are shown in Fig.2.

3. Conclusion

Phonons play a major role in many physical and electrical properties of condensed matter, such as thermal and electrical conductivity. The calculation of phonon dispersion curves is an important part of condensed matter studies. Material properties such as thermal capacity and conduction, phonon density of states, electrical conduction and mobility directly depend on finding phonon dispersion curves. In this paper, using discretization, and a new proposed technique, the resulted motion equations were converted to an eigenvalue problem. The results were presented as dispersion curves for shear, dilatational, and flexural modes of phonons.

References

[1] Alizadeh,A. et al., (2014), Tailoring electronphonon interaction in nanostructures, J. Photonics and Nanostructures - Fundamentals and Applications, 12(2), pp.164172.

[2] Balandin,A.A., Pokatilov,E.P., and Nika,D.L., (2007), Phonon Engineering in Hetero and Nanostructures, J. Nanoelectronics and Optoelectronics, (2), pp.140170.

[3] Rostami,A., Alizadeh,A., Baghban H., Alizadeh,T., and Bahar,H.B., (2011), Phonon engineering in nanoscale layered structures, SPIE (7987), 79870F-79871F.

[4] Pokatilov,E.P., Nika,D.L., and Balandin,A.A., (2003), Phonon spectrum and group velocities in AlN/GaN/AlN and related heterostructures, Superlattices Microstruct., (33), pp.155171.

[5] Balandin,A.A., Nika,D.L., and Pokatilov,E.P., (2004), Phonon spectrum and group velocities in wurtzite hetero-structures, phys. stat. sol., 1(11), pp.26582661.

[6] Wright,A.F., (1997), Elastic properties of zinc-blende and wurtzite AlN, GaN, and InN, J. Appl. Phys., 82(2833).

[7] Marasi,H.R. and Pourmostafa Aqdam,A., (2015), Homotopy analysis method and homotopy Pade approximants for solving the FornbergWhitham equation, Eurasian Math. J., 6(1), pp.65-75.

[8] Marasi,H.R. and Khezri,E., (2014), Asymptotic distributions of Neumann problem for Sturm-Liouville equation Computational methods for differential equational, 2(1), pp.19-25.

[9] Mishra,L.N., Agarwal R.P., and Sen,M., (2016), Solvability and asymptotic behavior for some nonlinear quadratic integral equation involving Erdélyi-Kober fractional integrals on the unbounded interval, Progress in Fractional Differentiation and Applications, 2(3), pp.153-168.

[10] Mishra,L.N., and Agarwal,R.P., (2016), On existence theorems for some nonlinear functional-integral equations, Dynamic Systems and Applications, 25, pp.303-320.

[11] Mishra,V.N., (2007), Some Problems on Approximations of Functions in Banach Spaces, Ph.D. Thesis, Indian Institute of Technology, Roorkee 247 667, Uttarakhand, India.

[12] Gandhi,R.B. and Mishra, V.N.,(2016), Local and global results for modified Szász - Mirakjan operators, Math. Method. Appl. Sci. DOI: 10.1002/mma.4171.

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