# LATTICE THEORY OF SHEAR MODES OF VIBRATION AND TORSIONAL EQUILIBRIUM OF SIMPLE-CUBIC CRYSTAL PLATES AND BARS

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Abstract—With a view toward helping to bridge the gap, from the discrete side, between discrete and continuum models of crystalline, elastic solids, analytic solutions, in closed form, are obtained of the Gazis–Herman–Wallis finite difference equations of a simple-cubic, crystal lattice for the cases of thickness-shear vibrations of a plate, face-shear and thickness-twist waves in a plate, axial shear vibrations of a rectangular bar and torsional equilibrium of a rectangular bar. The simple character of the solutions facilitates detailed studies of frequencies and deformations as the dimensions of the bodies and the wave lengths (or the dimensions alone, in the case of equilibrium) increase from interatomic distances to the sizes at which the classical continuum theory may be used.

#### **INTRODUCTION**

It is known that the description of the motions of elastic solids, by means of the classical theory of the elastic continuum, is limited to bodily dimensions and wave lengths large in comparison with a representative dimension of the structure of the material. Estimates of the magnitudes of the errors, as wave lengths and sizes diminish to structural dimensions, require data outside the compass of classical elasticity. One source of such data, applicable to crystalline solids, is the dynamical theory of crystal lattices [1]. The difference equations and boundary conditions of lattice theory have, as their long wave, low frequency limit, the differential equations and boundary conditions of classical elasticity. Analogous lattice and continuum solutions of vibration and wave propagation problems, or problems of equilibrium, for bodies with at least one finite dimension, can be used to calculate the errors in the continuum solutions as dimensions or wave lengths approach interatomic distances. Comparisons between the two types of solution are simplified if both are expressed in simple terms. In classical elasticity there are many such simple examples for bodies with one or two pairs of parallel, free boundaries; but analogous solutions of the difference equations of crystal lattice theory are rare.

The difference equations employed in this study are those formulated by Gazis, Herman and Wallis [2] for a simple-cubic lattice with nearest and next nearest neighbor central force interactions and angular interactions between three, successive, non-collinear atoms. Simple-cubic is the simplest of all lattice structures and the Gazis–Herman–Wallis equations are the simplest lattice equations that do not require a relation among the three elastic constants of cubic symmetry. Although no natural crystals with simple-cubic structure are known to exist, the idea is a suitable one for the present study.

Four problems are considered: Thickness-shear vibrations of a plate, face-shear and thickness-twist waves in a plate, axial shear vibrations of a rectangular bar and torsional equilibrium of a rectangular bar. In all cases, the faces of the plate or bar are free of traction.

The solutions are known, simple ones in classical elasticity and almost equally simple, analogous solutions of the lattice equations are derived, here, for comparison.

In the case of the vibration and wave propagation problems, explicit, closed, analytic solutions of the difference equations and boundary conditions are obtained straight-forwardly. In the problem of torsional equilibrium of a rectangular bar, a complication is encountered, at an intermediate stage of solution, in the form of a system of simultaneous, linear, algebraic equations for the coefficients of a finite series representation of the warping function. The number of equations is equal to half the number of atoms (for an even number of atoms) or half the number of spaces between atoms (for an odd number of atoms) along one side of the cross section. However, an explicit solution is obtained for the typical unknown of the system of equations so that the final expression for the warping function is also an explicit, closed, analytic one.

In general, it is found that wave lengths or dimensions do not have to be greater than about half a dozen times the distance between nearest neighbor atoms for the continuum theory to be adequate. However, marked differences between analogous lattice and continuum solutions occur for smaller wave lengths or dimensions.

#### DIFFERENCE EQUATIONS OF MOTION AND BOUNDARY CONDITIONS

In rectangular coordinates x, y, z, the atoms of a simple-cubic, crystal lattice are taken to be at points x = la, y = ma, z = na, where l, m, n are positive or negative integers and a is the distance between nearest neighbor atoms. The force constants between nearest neighbors and between next nearest neighbors are designated by  $\alpha$  and  $\beta$ , respectively, while  $\gamma$  is the angular force constant between three, successive, non-collinear atoms. Then, if  $u_{l,m,n}$ ,  $v_{l,m,n}$ ,  $w_{l,m,n}$  are the rectangular components of displacement of the atom at point l, m, n, Gazis, Herman and Wallis [2] find three equations of motion of the type

$$\alpha(u_{l+1,m,n} + u_{l-1,m,n} - 2u_{l,m,n}) + \beta(u_{l+1,m+1,n} + u_{l-1,m-1,n} + u_{l+1,m+1,n} + u_{l+1,m,n+1} + u_{l-1,m,n-1} + u_{l+1,m,n-1} + u_{l+1,m,n-1} + u_{l-1,m,n+1}) + (\beta + \gamma)(v_{l+1,m+1,n} + v_{l-1,m-1,n} - v_{l+1,m-1,n} - v_{l-1,m+1,n} + w_{l+1,m,n+1} + w_{l-1,m,n-1} \quad (1) - w_{l+1,m,n-1} - w_{l-1,m,n+1}) + 4\gamma(u_{l,m+1,n} + u_{l,m-1,n} + u_{l,m,n-1} - 4u_{l,m,n}) = \rho a^{3}\ddot{u}_{l,m,n},$$

where  $\rho a^3$  is the mass of an atom. The remaining two equations of motion are obtained by cyclical permutation of u, v, w and l, m, n.

At free boundaries  $l = \pm L$ , the conditions to be satisfied are

$$\pm \alpha(u_{\pm(L+1),m,n} - u_{\pm L,m,n})$$

$$\pm \beta(u_{\pm(L+1),m+1,n} + u_{\pm(L+1),m-1,n} + u_{\pm(L+1),m,n+1} + u_{\pm(L+1),m,n-1} - 4u_{\pm L,m,n})$$

$$+ \beta(v_{\pm(L+1),m+1,n} - v_{\pm(L+1),m-1,n} + w_{\pm(L+1),m,n+1} - w_{\pm(L+1),m,n-1})$$

$$\pm 2\gamma(u_{\pm L,m+1,n} + u_{\pm L,m-1,n} + u_{\pm L,m,n+1} + u_{\pm L,m,n-1} - 4u_{\pm L,m,n})$$

$$+ \gamma(v_{\pm(L+1),m+1,n} - v_{\pm(L+1),m-1,n} - v_{\pm L,m+1,n} + v_{\pm L,m-1,n})$$

$$+ \gamma(w_{\pm(L+1),m,n+1} - w_{\pm(L+1),m,n-1} - w_{\pm L,m,n+1} + w_{\pm L,m,n-1}) = 0,$$

$$\pm \beta(v_{\pm(L+1),m+1,n} + v_{\pm(L+1),m-1,n} - 2v_{\pm L,m,n}) + \beta(u_{\pm(L+1),m+1,n} - u_{\pm(L+1),m-1,n}) \pm 4\gamma(v_{\pm(L+1),m,n} - v_{\pm L,m,n}) + \gamma(u_{\pm(L+1),m+1,n} - u_{\pm(L+1),m-1,n} + u_{\pm L,m+1,n} - u_{\pm L,m-1,n}) = 0, \pm \beta(w_{\pm(L+1),m,n+1} + w_{\pm(L+1),m,n-1} - 2w_{\pm L,m,n}) + \beta(u_{\pm(L+1),m,n+1} - u_{\pm(L+1),m,n-1}) \pm 4\gamma(w_{\pm(L+1),m,n} - w_{\pm L,m,n}) + \gamma(u_{\pm(L+1),m,n+1} - u_{\pm(L+1),m,n-1} + u_{\pm L,m,n+1} - u_{\pm L,m,n-1}) = 0.$$

Although solutions are given, in the sequel, only for odd numbers of atoms between boundaries, the solutions for even numbers can be obtained in a similar manner.

## THICKNESS-SHEAR VIBRATIONS OF A PLATE

In a plate bounded by  $l = \pm L$ , consider displacements

$$u_{l,m,n} = v_{l,m,n} = 0,$$
  

$$w_{l,m,n} = (A_1 \cos \xi la + A_2 \sin \xi la) e^{i\omega t}, \qquad 0 \leqslant \xi a \leqslant \pi.$$
(3)

With these displacements, the first two equations of the type (1) are satisfied identically and the third is satisfied if

$$\rho a^2 \omega^2 = 4\mu \sin^2 \frac{1}{2} \xi a,\tag{4}$$

where

$$\mu = 2(\beta + 2\gamma)/a. \tag{5}$$

Upon substituting the displacements (3) in the boundary conditions (2), we find that the first two conditions are satisfied identically and the third is satisfied if

$$\xi a = p\pi/(2L+1), \qquad p = 0, 1, 2, \dots, < 2L+1,$$
 (6)

where even and odd p apply to symmetric and antisymmetric modes, respectively. Thus, the frequencies are

$$\omega = \frac{2}{a} \left( \frac{\mu}{\rho} \right)^{\frac{1}{2}} \sin \frac{p\pi}{2(2L+1)}, \qquad p = 0, 1, 2, \dots, < 2L+1,$$
(7)

and the displacements are

$$w_{l,m,n} = \left(A_1 \cos \frac{p\pi l}{2L+1} + A_2 \sin \frac{p\pi l}{2L+1}\right) e^{i\omega t}.$$
 (8)

To compare the solution with the continuum one, we consider a continuum plate of thickness 2h, where

$$2h = (2L+1)a,\tag{9}$$

i.e. each layer of atoms is replaced by a continuum layer of thickness a. The frequencies of the thickness-shear modes of such a plate are given by

$$\omega = (p\pi/2h)(\mu/\rho)^{\frac{1}{2}}, \qquad p = 0, 1, 2, \dots,$$
(10)

and the displacements are

$$w = [A_1 \cos(p\pi x/2h) + A_2 \sin(p\pi x/2h)] e^{i\omega t}.$$
 (11)

In the long wave, low frequency approximation  $(la \rightarrow x, p \leq 2L+1)$ , it may be seen that (7) and (8) approach (10) and (11), respectively.

If the frequency for p = 1, in (10), i.e.

$$\omega_1 = \frac{\pi}{2h} \left( \frac{\mu}{\rho} \right)^{\frac{1}{2}} = \frac{\pi}{(2L+1)a} \left( \frac{\mu}{\rho} \right)^{\frac{1}{2}},$$
(12)

is used as a reference frequency, the normalized frequencies for the lattice are

$$\Omega = \frac{\omega}{\omega_1} = \frac{2(2L+1)}{\pi} \sin \frac{p\pi}{2(2L+1)}, \qquad p = 0, 1, 2, \dots, < 2L+1,$$
(13)

and these are to be compared with the normalized frequencies, p, for the continuum.

The normalized frequencies of the lattice are given in Table 1 for plates 1, 3, 5, ..., 15 atomic layers thick. It may be seen how, for a mode of any order p > 0, the normalized frequencies approach the normalized frequency, p, of the continuum as the number of layers increases. Also, as the number of layers increases, the number of lower modes that have frequencies nearly equal to those of the corresponding modes of the continuum increases. For a given number of layers, the discrepancy between the frequencies of the lattice and the continuum increases as the order of the mode increases. The corresponding

Table 1. Normalized frequencies,  $\Omega$ , of thickness-shear modes of vibration, of order p, in plates 2L+1atomic layers thick

	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7
p = 0	0	0	0	0	0	0	0	0
p = 1		0.955	0.984	0.990	0.995	0.997	0.998	0.998
p = 2		1.654	1.871	1.934	1.960	1.972	1.978	1.985
p = 3			2.575	2.778	2.865	2.909	2.935	2.951
p = 4			3.027	3.484	3.683	3.786	3.845	3.884
p = 5				4.015	4.389	4.586	4.701	4·775
p = 6				4.344	4.962	5.292	5-488	5.613
p = 7					5.385	5.891	6.196	6.390
p = 8					5.643	6.370	6.811	7.097
p = 9						6.719	7.328	7.726
p = 10						6.932	7.738	8.270
p = 11							8.038	8.724
p = 12							8.216	9.082
p = 13								9.340
p = 14								9.497

departure of the lattice mode-shape from the sinusoidal form of the continuum mode is illustrated, for the case of fifteen layers, in Fig. 1. It may be seen that, for the first few modes, where the lattice mode-shapes are nearly sinusoidal, the normalized frequencies p and  $\Omega$ are nearly the same; but, as the mode shape departs from sinusoidal for increasing orders, the frequencies separate—by almost 50 per cent for the highest mode, in this case. As the number of layers increases, the discrepancy between the frequencies of the highest lattice



FIG. 1.

mode and the corresponding continuum mode approaches  $(50\pi-100)$  per cent. It should be noted that, whereas the number of modes in the continuum is unlimited, the number of modes in the lattice is equal to the number of layers. A wave described by N points can have no more than N-1 nodes.

### FACE-SHEAR AND THICKNESS-TWIST WAVES IN A PLATE

Waves, in a plate, with displacement and wave normal at right angles to each other and parallel to the faces of the plate, are called thickness-twist waves except for the wave of zero order (in which the displacement does not vary through the thickness of the plate) which is called a face-shear wave. In the lattice plate considered in the preceding section, such waves are represented by displacements of the form

$$u_{l,m,n} = v_{l,m,n} = 0,$$

$$w_{l,m,n} = (A_1 \cos \xi la + A_2 \sin \xi la) e^{i(\eta m a - \omega t)} \begin{cases} 0 \leqslant \xi a \leqslant \pi, \\ 0 \leqslant \eta a \leqslant \pi. \end{cases}$$
(14)

This time, the equations of motion require

$$\rho a^2 \omega^2 = 4\mu (\sin^2 \frac{1}{2}\xi a + \sin^2 \frac{1}{2}\eta a)$$
(15)

and the boundary conditions again require (6). Thus, the normalized frequencies are

$$\Omega = \frac{\omega}{\omega_1} = \frac{2(2L+1)}{\pi} \left( \sin^2 \frac{p\pi}{2(2L+1)} + \sin^2 \frac{1}{2} \eta a \right)^{\frac{1}{2}}, \qquad p = 1, 2, \dots, < 2L+1, \quad (16)$$

and the displacements are

$$w_{l,m,n} = \left(A_1 \cos \frac{p\pi l}{2L+1} + A_2 \sin \frac{p\pi l}{2L+1}\right) e^{i(\eta m a - \omega t)}.$$
 (17)

In the long wave, low frequency limit  $(la \rightarrow x, ma \rightarrow y, p \ll 2L+1)$ , these become the known results from elasticity theory:

$$\Omega = [p^2 + (2\eta h/\pi)^2]^{\frac{1}{2}}, \qquad p = 0, 1, 2, \dots,$$
(18)

$$w = [A_1 \cos(p\pi x/2h) + A_2 \sin(p\pi x/2h)] e^{i(\eta y - \omega t)}.$$
 (19)

The real branches of the dispersion relation (16), for the lattice, are illustrated, in Fig. 2, for a plate fifteen layers thick (L = 7). At infinite wave length  $(\eta = 0)$  along the plate, the modes reduce to the thickness-shear modes illustrated in Fig. 1. These variations across the thickness of the plate are maintained for all wave lengths,  $2\pi/\eta$ , along the plate. The major differences between the dispersion relations for the lattice and the continuum are: Each of the finite number, 2L+1, of branches of the lattice dispersion relation (16) has a high frequency cutoff, in addition to a low frequency cutoff (13), and all have the same upper cutoff,  $\eta = \pi/a$ , of wave number, i.e. wave length equal to 2a; whereas all the infinity of real branches of the continuum dispersion relation (18) are hyperbolic curves extending from low frequency cutoffs, at  $\eta = 0$ ,  $\Omega = 1, 2, ..., \infty$ , to infinite frequencies and wave numbers—asymptotic to

$$\Omega = (2L+1)\eta a/\pi, \tag{20}$$



which is a straight line starting from the lower left corner and passing through the upper right corner of Fig. 2 and is, in fact, the face-shear branch of the continuum dispersion relation. Thus, the dispersion relation for the continuum is a good approximation to that for the lattice only in the lower left hand region of Fig. 2; i.e. for long wave lengths, in comparison with *a*, both along the plate and across its thickness. For any given order of mode (p < 2L+1), wave length  $(2\pi/\eta)$  and thickness (2h = [2L+1]a) or number of layers, the error in the continuum approximation may be found, readily, by comparing (18) and (19) with (16) and (17).

As in the case of the continuum, the lattice dispersion relation has branches for real frequency and imaginary wave number which are not shown in Fig. 2.

## AXIAL SHEAR VIBRATIONS OF A RECTANGULAR BAR

We consider a bar bounded by  $l = \pm L$ ,  $m = \pm M$ , with displacements

$$u_{l,m,n} = v_{l,m,n} = 0,$$

$$w_{l,m,n} = (A_1 \cos \xi la \sin \eta ma + A_2 \sin \xi la \sin \eta ma) e^{i\omega t}$$

+  $(A_3 \cos \xi la \cos \eta ma + A_4 \sin \xi la \cos \eta ma) e^{i\omega t}$ .

Upon substituting these displacements in the equations of motion (1) and the boundary conditions (2), we again find (15) and (6). The boundary conditions at  $m = \pm M$  are obtained from (2) by one cyclical permutation of u, v, w and l, m, n. Substitution of (21) in the result yields

$$\eta a = q\pi/(2M+1), \qquad q = 0, 1, 2, \dots, < 2M+1.$$
 (22)

(21)

Hence, the normalized frequencies of axial shear vibrations of the rectangular bar are given by

$$\Omega = \frac{2(2L+1)}{\pi} \left( \sin^2 \frac{p\pi}{2(2L+1)} + \sin^2 \frac{q\pi}{2(2M+1)} \right)^{\frac{1}{2}} \begin{cases} p = 0, 1, 2, \dots, < 2L+1, \\ q = 0, 1, 2, \dots, < 2M+1, \end{cases}$$
(23)

i.e. simply by the replacement of  $\eta a$ , in (16), by its values (22). For a bar with a cross section 2L+1 atoms deep and 2M+1 atoms wide, the frequency of any mode with p nodes across the depth and q nodes across the width is readily calculated from (23). The total number of modes is equal to the number of atoms in the cross section.

If p/(2L+1) and q/(2M+1) become small enough, the frequencies approach the continuum limit

$$\Omega = (p^2 + q^2 h_1^2 / h_2^2)^{\frac{1}{2}}, \qquad p, q = 0, 1, 2, \dots,$$
(24)

where  $h_1$  and  $h_2$  are the half-depth and half-width, respectively, of the cross section.

To see how the frequencies vary in a bar fifteen atoms deep and any number of atoms wide, enter Fig. 2 at abscissa q/(2M+1) and note the frequencies for the branches p = 0, ..., 14 at that abscissa. As the ratio of the number, q, of nodes across the width to the number, 2M+1, of atoms across the width diminishes, the abscissa at entry is displaced to the left and the frequencies become lower. If, simultaneously, the ratio of the number, p, of nodes across the depth to the number, 2L + 1, of atoms across the depth diminishes, the frequencies approach the continuum limit (24).

#### TORSIONAL EQUILIBRIUM OF A RECTANGULAR BAR

The bar is bounded by free faces at  $l = \pm L$  and  $m = \pm M$  and is in equilibrium under a twist about the axis of z with angle of twist  $\tau$  per unit length.

By analogy with the St. Venant solution of the equations of classical elasticity for the analogous problem [3], it is assumed that

$$u_{l,m,n} = u_{m,n} = -\tau a^2 mn,$$

$$v_{l,m,n} = v_{l,n} = \tau a^2 ln,$$

$$w_{l,m,n} = w_{l,m} = \tau a^2 (lm + A \sin l\theta \sinh m\varphi), \qquad 0 < \theta < \pi.$$
(25)

With these displacements, the first two equations of the type (1), with the right hand side zero, are satisfied identically and the third equation is satisfied if

$$\cosh \varphi = 2 - \cos \theta. \tag{26}$$

The conditions of the type (2), for free boundaries, reduce, in view of (25), to

$$\pm 2(w_{\pm (L+1),m} - w_{\pm L,m}) + u_{m,n+1} - u_{m,n-1} = 0 \quad \text{on} \quad l = \pm L, \tag{27}$$

$$\pm 2(w_{l,\pm(M+1)} - w_{l,\pm M}) + v_{l,n+1} - v_{l,n-1} = 0 \quad \text{on} \quad m = \pm M.$$
(28)

Upon substituting (25) in (27), we find

$$\theta = \theta_p = (2p-1)\pi/(2L+1), \quad p = 1, 2, \dots, L.$$
 (29)

Hence, the third of (25) may be written as a finite series :

$$w_{l,m} = \tau a^2 \left( lm + \sum_{p=1}^{p=L} A_p \sin l\theta_p \sinh m\varphi_p \right).$$
(30)

Substitution of (30) in the boundary conditions (28) yields

$$\sum_{p=1}^{p=L} A_p \sin l\theta_p \sinh \frac{1}{2} \varphi_p \cosh(M + \frac{1}{2}) \varphi_p = -l, \qquad l = 1, 2, \dots, L,$$
(31)

i.e. a set of L simultaneous, linear, algebraic equations on the coefficients  $A_p$ . The system of equations can be solved explicitly for the  $A_p$  by a method analogous to that for determining Fourier coefficients. Multiply both sides of (31) by  $\sin l\theta_q$  and sum over l from l = 1 to l = L. Now [4],

$$\sum_{l=1}^{l=L} l \sin l\theta_{p} = \frac{\sin L\theta_{p}}{4\sin^{2}\frac{1}{2}\theta_{p}} - \frac{L\cos(L+\frac{1}{2})\theta_{p}}{2\sin\frac{1}{2}\theta_{p}}.$$
(32)

Also, employing (29), we find

$$\sum_{l=1}^{l=L} \sin l\theta_p \sin l\theta_q = \begin{cases} 0, & q \neq p, \\ \frac{1}{4}(2L+1), & q = p. \end{cases}$$
(33)

Hence:

$$A_p = \frac{2L\sin\frac{1}{2}\theta_p \cos(L+\frac{1}{2})\theta_p - \sin L\theta_p}{(2L+1)\sinh^3\frac{1}{2}\varphi_p \cosh(M+\frac{1}{2})\varphi_p}.$$
(34)

Substitution of (34) in (30) completes the solution for the warping function  $w_{l,m}$ .

The approach of the warping from shapes peculiar to the lattice to the shapes, depicted in Figs. 3 and 4, found in the St. Venant solution for the continuum, is illustrated by a few



FIG. 3.



Fig. 4.

examples of  $w_{l,m}$  for successively larger cross sections. First, for L = 1, M = 1, 2, 3, 4, we find

$$L = 1, M = 1: \quad w_{0,0} = w_{0,\pm 1} = w_{\pm 1,0} = 0$$
  

$$w_{1,1} = w_{-1,-1} = w_{1,-1} = w_{-1,1} = 0$$
  

$$L = 1, M = 2: \quad w_{0,0} = w_{0,\pm 1} = w_{0,\pm 2} = w_{\pm 1,0} = 0$$
  

$$w_{1,1} = w_{-1,-1} = -w_{1,-1} = -w_{-1,1} = 3\tau a^{2}/5$$
  

$$w_{1,2} = w_{-1,-2} = -w_{1,-2} = -w_{-1,2} = 4\tau a^{2}/5$$
  

$$L = 1, M = 3: \quad w_{0,0} = w_{0,\pm 1} = w_{0,\pm 2} = w_{0,\pm 3} = w_{\pm 1,0} = 0$$
  

$$w_{1,1} = w_{-1,-1} = -w_{1,-1} = -w_{-1,1} = 11\tau a^{2}/13$$
  

$$w_{1,2} = w_{-1,-2} = -w_{1,-2} = -w_{-1,2} = 20\tau a^{2}/13$$
  

$$w_{1,3} = w_{-1,-3} = -w_{1,-3} = -w_{-1,3} = 23\tau a^{2}/13$$
  

$$L = 1, M = 4: \quad w_{0,0} = w_{0,\pm 1} = w_{0,\pm 2} = w_{0,\pm 3} = w_{0,\pm 4} = w_{\pm 1,0} = 0$$

= 1, 
$$M = 4$$
:  $w_{0,0} = w_{0,\pm 1} = w_{0,\pm 2} = w_{0,\pm 3} = w_{0,\pm 4} = w_{\pm 1,0} = 0$   
 $w_{1,1} = w_{-1,-1} = -w_{1,-1} = -w_{-1,1} = 16\tau a^2/17$   
 $w_{1,2} = w_{-1,-2} = -w_{1,-2} = -w_{-1,2} = 31\tau a^2/17$   
 $w_{1,3} = w_{-1,-3} = -w_{1,-3} = -w_{-1,3} = 43\tau a^2/17$   
 $w_{1,4} = w_{-1,-4} = -w_{1,-4} = -w_{-1,4} = 47\tau a^2/17.$ 

These displacements are displayed in Fig. 5.

It may be seen that, with one dimension of the cross section restricted to three layers of atoms (L = 1), the warping bears little resemblance to that found by St. Venant; namely there is no warping of the square section (L = 1, M = 1) and, in each succeeding section, the displacements at a long side  $(l = \pm 1, m = 0, \pm 1, \pm 2, ...)$  do not have a maximum and a minimum between the center and the ends, as they have in the continuum solution illustrated in Figs. 3 and 4. In fact, it may be shown that, for L = 1 and l = 1,

$$\frac{w_{1,m}}{\tau a^2} = m - \frac{2^{M-m+2} [(3+\sqrt{5})^m - (3-\sqrt{5})^m]}{(1+\sqrt{5})(3+\sqrt{5})^M - (1-\sqrt{5})(3-\sqrt{5})^M},$$
(35)

which is a monotonically increasing function of m, from zero to M, for any M.

However, for L = 2, M = 2, 3, ..., the dissimilarity disappears. We have:

$$L = 2, M = 2: \quad w_{0,0} = w_{0,\pm 1} = w_{0,\pm 2} = w_{\pm 1,0} = w_{\pm 2,0} = 0$$
$$w_{1,\pm 1} = w_{-1,\pm 1} = w_{2,\pm 2} = w_{-2,\pm 2} = 0$$
$$w_{2,1} = w_{-1,2} = w_{-2,-1} = w_{1,-2} = \tau a^2/3$$
$$w_{1,2} = w_{-2,1} = w_{-1,-2} = w_{2,-1} = -\tau a^2/3$$

$$L = 2, M = 3: \quad w_{0,0} = w_{0,\pm 1} = w_{0,\pm 2} = w_{0,\pm 3} = w_{\pm 1,0} = w_{\pm 2,0} = 0$$
  

$$w_{1,1} = w_{-1,-1} = -w_{1,-1} = -w_{-1,1} = 121\tau a^{2}/281$$
  

$$w_{1,2} = w_{-1,-2} = -w_{1,-2} = -w_{-1,2} = 184\tau a^{2}/281$$
  

$$w_{1,3} = w_{-1,-3} = -w_{1,-3} = -w_{-1,3} = 117\tau a^{2}/281$$
  

$$w_{2,1} = w_{-2,-1} = -w_{2,-1} = -w_{-2,1} = 300\tau a^{2}/281$$
  

$$w_{2,2} = w_{-2,-2} = -w_{2,-2} = -w_{-2,2} = 498\tau a^{2}/281$$
  

$$w_{2,3} = w_{-2,-3} = -w_{2,-3} = -w_{-2,3} = 448\tau a^{2}/281$$

$$L = 2, M = 4: \quad w_{0,0} = w_{0,\pm 1} = w_{0,\pm 2} = w_{0,\pm 3} = w_{0,\pm 4} = w_{\pm 1,0} = w_{\pm 2,0} = 0$$

$$w_{1,1} = w_{-1,-1} = -w_{1,-1} = -w_{-1,1} = \frac{1539\tau a^2}{2245}$$

$$w_{1,2} = w_{-1,-2} = -w_{1,-2} = -w_{-1,2} = \frac{2814\tau a^2}{2245}$$

$$w_{1,3} = w_{-1,-3} = -w_{1,-3} = -w_{-1,3} = \frac{3475\tau a^2}{2245}$$

$$w_{1,4} = w_{-1,-4} = -w_{1,-4} = -w_{-1,4} = \frac{3006\tau a^2}{2245}$$

$$w_{2,1} = w_{-2,-1} = -w_{2,-1} = -w_{-2,1} = \frac{3342\tau a^2}{2245}$$

$$w_{2,2} = w_{-2,-2} = -w_{2,-2} = -w_{-2,2} = 6242\tau a^2/2245$$
  

$$w_{2,3} = w_{-2,-3} = -w_{2,-3} = -w_{-2,3} = 8080\tau a^2/2245$$
  

$$w_{2,4} = w_{-2,-4} = -w_{2,-4} = -w_{-2,4} = 7788\tau a^2/2245$$

These displacements are displayed in Fig. 6.

0	<u>↓</u> 3	0	- 1/3	0					
	٥	0	0	<u> </u> 3					
o	o	o	0	0	L=	2, M	= 2		<u> </u>
1 3	o	٥	٥	$-\frac{1}{3}$					×
o	- 1/3	0	$\frac{1}{3}$	0					
440 281	4 <b>98</b> 281	300 281	0	- <mark>30</mark> 0 281	- <b>498</b> -281	-448			
<u>117</u> 281	184 281	121 281	0	- <mark>121</mark> 281	- 184	- <mark>117</mark> 281			
o	o	o	o	٥	0	0	L	= 2, M =	= 3
- <u>117</u> 281	- <u>184</u> 281	-121 281	0	1 <u>21</u> 28/	184 281	<u>117</u> 201			
- <u>448</u> 281	- 498 261	- <u>300</u> 281	0	300 281	498 281	448 281			
<u>7788</u> 2245	<u>8080</u> 2245	<u>6242</u> 2245	<u>3342</u> 2245	o	- <u>3342</u> 2245	<u>6242</u> 2245	8080 2245	7788	
<u>30,06</u> 22,45	3475 2245	2814 2245	15 <u>39</u> 2245	0	- 1539 2245	2814	3475 2245	3006 2245	
0	٥	0	o	o	0	0	o	o	L=2, M=4
3006 2245	- <u>3475</u> 2245	2814	1539 2248	0	1539 2245	2814 2245	<u>3475</u> 2245	3006 2245	
7788 2245	8080 2245	<u>6242</u> 2245	- <u>3342</u> 2245	o	3342 2245	6242 2245	8080 2245	7788 2245	
					Fic	3. 6.			

For the square (L = 2, M = 2), it may be seen that the cross section is divided into eight sectors, with alternating signs of displacement, instead of the usual four sectors for a long, rectangular section. This is precisely the result found by St. Venant for the continuum, as illustrated in Fig. 4. For the rectangular sections L = 2, M = 3 and L = 2, M = 4, the displacements along a long side reach a maximum and a minimum, near the ends, while, along a short side, the displacements vary monotonically. Again, these results are the same as the corresponding ones in St. Venant's solution, as illustrated in Fig. 3. Thus, the cross section need have only as many as five atoms along the shorter side for the warping function to have all the qualitative properties found in the continuum solution. It may be observed that, for both L = 1 and L = 2, the normalized axial displacements,  $w_{l,m}/\tau a^2$ , are expressed simply as ratios of integers. This is made possible by the fact that trigonometric functions of

$$\theta_p = (2p-1)\pi/(2L+1), \qquad p = 1, 2, \dots, L,$$
 (29)

can be expressed in closed, algebraic form if L = 1 or L = 2. Thus, for

$$L = 1: \cos \theta_1 = \cos(\pi/3) = \frac{1}{2};$$
 (36)

$$L = 2: \quad \cos \theta_1 = \cos(\pi/5) = \frac{1}{4}(\sqrt{(5)} + 1), \\ \cos \theta_2 = \cos(3\pi/5) = -\frac{1}{4}(\sqrt{(5)} - 1).$$
(37)

The next larger value of L for which such expressions are known is L = 7:

$$\cos \theta_{1} = \cos(\pi/15) = \frac{1}{8}(\sqrt{(5)} - 1) + \frac{1}{8}\sqrt{[6\sqrt{(5)}(\sqrt{(5)} + 1)]},$$
  

$$\cos \theta_{2} = \cos(3\pi/15) = \frac{1}{4}(\sqrt{(5)} + 1),$$
  

$$\cos \theta_{3} = \cos(5\pi/15) = \frac{1}{2},$$
  

$$\cos \theta_{4} = \cos(7\pi/15) = -\frac{1}{8}[\sqrt{(5)} + 1] + \frac{1}{8}\sqrt{[6\sqrt{(5)}(\sqrt{(5)} - 1)]},$$
  

$$\cos \theta_{5} = \cos(9\pi/15) = -\frac{1}{4}[\sqrt{(5)} - 1],$$
  

$$\cos \theta_{6} = \cos(11\pi/15) = \frac{1}{8}[\sqrt{(5)} - 1] - \frac{1}{8}\sqrt{[6\sqrt{(5)}(\sqrt{(5)} + 1)]},$$
  

$$\cos \theta_{7} = \cos(13\pi/15) = -\frac{1}{8}[\sqrt{(5)} + 1] - \frac{1}{8}\sqrt{[6\sqrt{(5)}(\sqrt{(5)} - 1)]}.$$

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Абстракт—Для устранения разниц, со стороны дискретных систем, между дискретной и сплошной моделью кристаллических, упругих тел, получаются аналитические решения, в замкнутом виде, для уравнения Газиса-Германа-Валлиса в конечных разностях, описывающие поведение простой кубической, кристаллической решетки. Этие решения касаются случая сдвиговых колебаний пластинки, поверхностных сдвиговых и крутильных волн в пластинке, осевых сдвиговых колебаний прямоугольного сечения и крутильного равновесия прямоугольного стержня. Простой характер решений, облегчает подробные исследования частот и деформаций, если размеры тел и длины волн /или только размеры, в случае равновесия/ увеличиваются от междуатомных размеров к размерам, при которых можно пользоваться классической теорией сплошной среды.