A COMPARISON OF DISCRETE AND CONTINUUM MODELS OF AN EDGE DISLOCATION IN A RECTANGULAR SIMPLE CUBIC CRYSTAL

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Edward M. Schall

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This is to certify that the

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EDWARD M. SCHALL

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ABSTRACT

A COMPARISON OF DISCRETE AND CONTINUUM MODELS
OF AN EDGE DISLOCATION IN A RECTANGULAR
SIMPLE CUBIC CRYSTAL

by Edward M. Schall

A single edge dislocation in a rectangularly bounded simple cubic crystal is simulated by two distinct models.

The first of these is a discrete lattice in which each nodal point is connected to its four nearest neighbors and its four next nearest neighbors in the plane by linear springs. An edge dislocation is introduced into an otherwise undisturbed lattice by placing a partial plane of lattice points between two existing full planes and then considering the springs which connect the extra plane lattice points to their neighbors to be held in a compressed configuration. This constraint is then removed and the strain energy initially concentrated in the springs of the extra plane of lattice points is distributed through the lattice displacing each point from its original position.

The second model is an elastic continuum into which a Volterra edge dislocation is introduced. The calculation of stresses and displacements requires the

superposition of an analytic solution which satisfies the displacement boundary condition and a numerical solution which satisfies the stress free condition on the rectangular boundaries of the continuum. In order to achieve elastic similarity so that corresponding results from the two models may be compared, it is necessary to use anisotropic elasticity theory for the continuum analysis.

Displacements for the two models are compared and the stresses of the continuum analysis are compared with analogous discrete quantities. These comparisons show that the results of the two models are remarkably similar. Corresponding values of the problem variables begin to differ appreciably only within four lattice spacings of the dislocation. Since the discrete model is a more physically correct means of describing the dislocation than the continuum model, this indicates that the continuum description may be accurately used at points which are much closer to the dislocation than the generally accepted value of ten lattice spacings.

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By

Edward M. Schall

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TABLE OF CONTENTS

LIST OF TABLES

List of Tables--Continued

LIST OF ILLUSTRATIONS

List of Illustrations--Continued

LIST OF APPENDICES

I. INTRODUCTION

In the more than thirty years since its origin, the theory of crystal dislocations has been successfully applied to many problems in the plastic deformation of crystalline solids. On the basis of dislocation theory reasonable physical explanations have been supplied for such experimentally observed phenomena as low mechanical strength, work hardening, annealing, and many others. Much of this theory has been of a qualitative nature, but that part which is quantitative has been, for the most part, derived from a material model which although it yields readily to mathematical analysis gives a rather poor description of the physical situation. This model is the elastic continuum and its mathematical key the theory of elasticity either anisotropic or more commonly isotropic.

The elastic dislocation as conceived by Volterra [1] and applied to the case of crystal dislocations by Cottrell [2] and others has the inherent disadvantage of describing a crystal defect which is atomic in nature by a model which is continuous. Even with such a serious shortcoming the continuum model of the crystal dislocation has been extensively used to determine stress

and displacement fields for such problems as isolated edge and screw dislocations, pairs of dislocations in proximity, arrays of dislocations with a common slip plane, dislocations in proximity with impurity atoms, dislocations near coated boundaries, and many other specific examples [2], [3].

All of these analyses possess the same essential weak points. These weak points may be emphasized by a consideration of the problem of a straight edge dislocation in terms of its description in the elastic dislocation theory. Referring to Figure 1 the physical description of this defect in a simple cubic lattice is that there is one more vertical plane of atoms above plane AA' than there is below it. What displacements then are necessary to mate the half plane above AA' to the half plane below it assuming that far away from the center of displacement the atomic planes such as BB' and CC' are completely lined up? The elastic dislocation which corresponds to this physical description is formed by cutting an elastic continuum along the plane OS in Figure 1 or Figure 2a and then displacing the adjacent faces of the cut by one atomic spacing, b, relative to one another, in the horizontal or x direction. To correspond to the symmetrical case shown in Figure 1 each face would be displaced by amount b/2 in opposite directions. The elasticity solution for the stress and strain fields in this problem is found for the isotropic case in Read [4] and for the anisotropic case in a paper by Eshelby [5]. Both

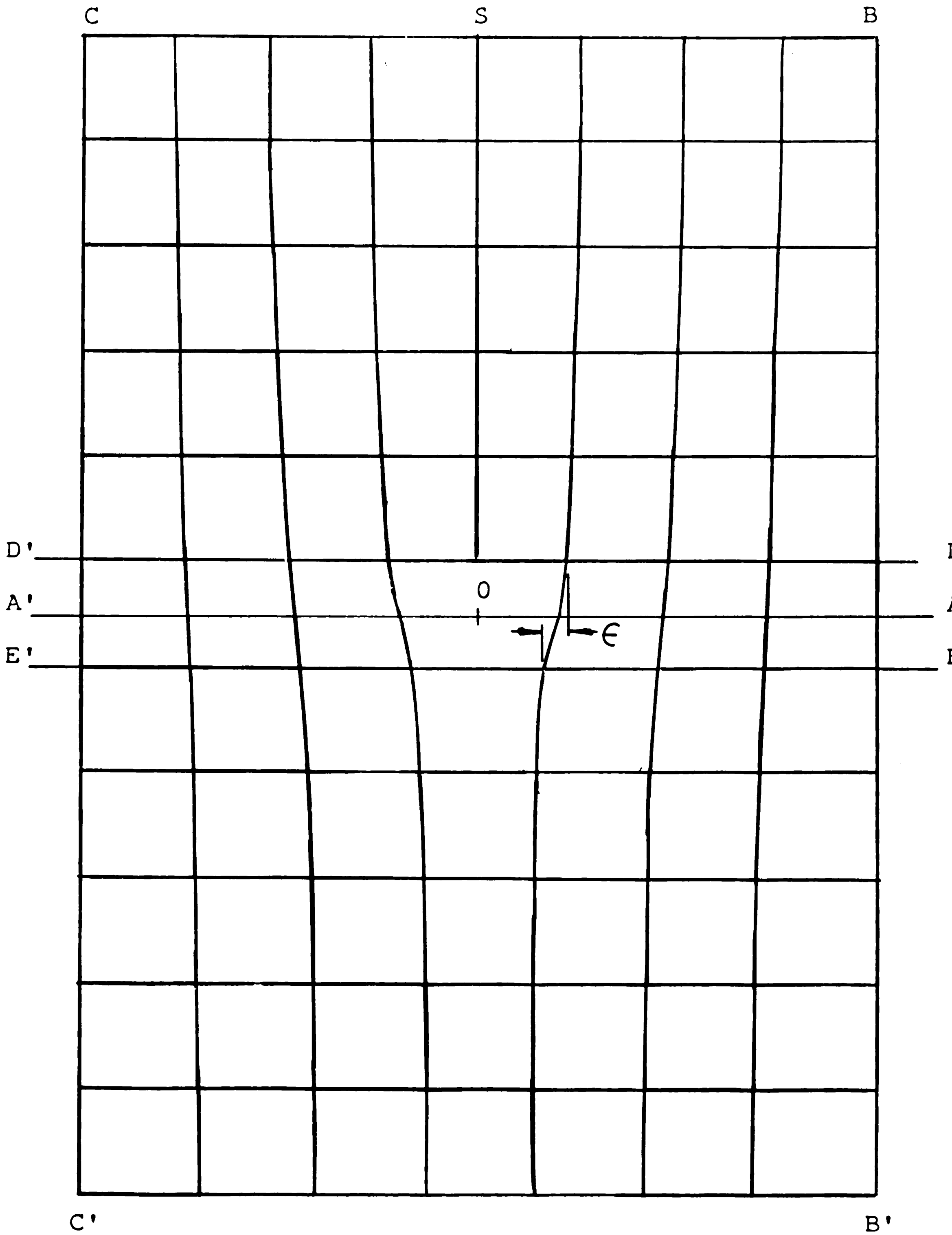
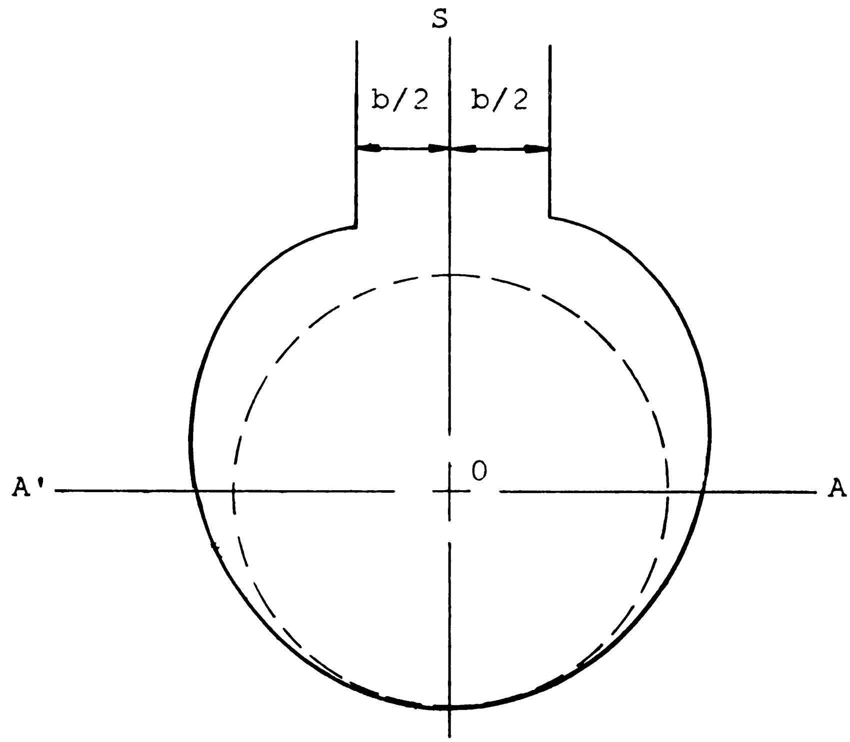
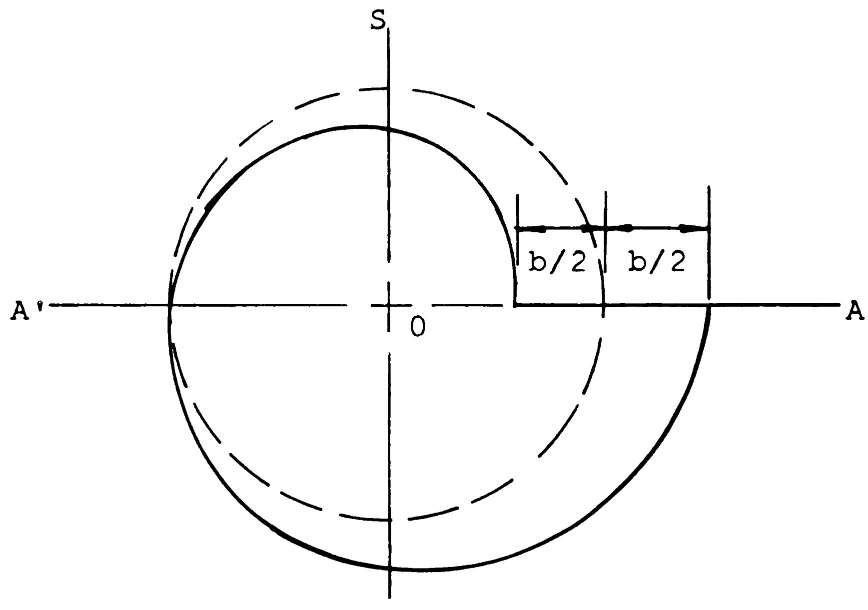


Fig. 1.--Physical appearance of a positive edge dislocation



(a)



(b)

Fig. 2.--Positive elastic edge dislocations

contain a singularity at the root of the cut, the point 0 in Figure 1 or Figure 2a, i.e., the stresses and strains are infinite here. For practical purposes a cylinder of material surrounding the point 0 in which stresses are too large to be legitimately described by an elastic analysis is also omitted from the region of the solution. Alternately the elastic edge dislocation may be constructed by cutting the continuum along the plane OA in Figure 1 or Figure 2b and displacing the opposite faces of the cut by the relative amount b as shown in Figure 2b.

The justification for the application of the elastic dislocation theory to describe the crystal dislocation is that for small relative atomic displacements the crystal lattice displacements and interatomic forces may be considered to be proportional. However, in the region close to the point 0 in Figure 1 where the relative atomic displacements are large the continuum model is completely unrealistic. The extent of the region in which the elastic continuum analysis is inapplicable is difficult to determine since it must depend on the characteristics of the atomic bond forces in this region, but a conservative estimate excludes a cylinder of about 10 atomic spacings [2].

Some attempts have been made to develop material models which may describe the region of a large deformation more realistically. Peierls [6], Nabarro [7], and Foreman [8] have described the edge dislocation in

Figure 1 in a way which takes some account of the atomic structure on the slip plane while assuming an elastic continuum elsewhere. They treat the problem as two elastic continua, one above the plane DD' and the other below the plane EE', in which the two planes exert a mutual periodic shear stress tending to compress the material above DD' and expand the material below EE'. The shear stress is a function of the relative displacement, ϵ , between corresponding points on DD' and EE' and is assumed to be a maximum when ϵ = b/2 and zero when ϵ = 0 so that the period of the shear stress is b. This model avoids the singularity encountered in the elastic dislocation analysis and uses a non-linear force displacement representation on the slip plane and especially in the region of high distortion. However, it assumes no displacement normal to the slip plane and also assumes that the only large deflections occur on the slip plane. This analysis indicates that the length of the slip plane over which the quantity ϵ is more than .25b is only 1.5b, i.e., the region of large deformation is 1.5b, for the case when the periodic shear force is a sine function. This appears to be a low estimate of the region of large deformation. By equating the potential energy change due to an infinitesimal displacement of the dislocation to the work done by the shear stress on the slip plane, Nabarro and Foreman have determined the shear stress which is necessary to cause the dislocation to propogate leaving slipped material in its wake. This stress is large if the region of large disturbance is confined to a small length of the slip plane and becomes smaller if the disturbance is spread out over a large length of the slip plane.

The actual atomic displacements for any real crystalline substance containing dislocations, at least in the region of high atomic misalignment, can only be found by a quantum mechanical analysis of the problem. This approach is prohibitively complex and must immediately be abandoned. The next simplest possibility would be to consider the atoms as particles which exert atomic forces on one another. But again the details of interatomic forces are to a large degree unknown and even simple models of these forces are mathematically complex for large atomic displacements. It is true, however, that material models using the interatomic force concept do exist which are still simple enough to be mathematically practical. Hopefully these models are closer to reality than those assuming the elastic continuum.

Such a simple atomic force model was used by Maradudin [9] to determine the displacements in an infinite crystal lattice due to the presence of a screw dislocation. His model consists of a simple cubic lattice in which each lattice point exerts a shearing force on its four nearest neighbors. This force is linearly proportional to the relative shearing motion of that lattice point with respect to each of its neighbors. For this particular case he is able to find an analytic function which satisfies the force equilibrium equations of all lattice points in the crystal. The displacements predicted from this analysis seem to be more realistic than those resulting from the elastic dislocation solution.

A somewhat similar material model of a crystal lattice, in this case bounded rather than infinite, is used in this thesis. An edge dislocation is introduced into the otherwise undisturbed and unloaded lattice and the resulting displacements are determined by the simultaneous solution of the force equilibrium equations for each lattice point.

As a comparison with the results of this analysis, a similar calculation is made for the case of an elastic dislocation. The material parameters and the geometry of both models are as similar as possible, to the extent of using cubic anisotropic elasticity for the continuum solution. The similarity of the two models is discussed in detail in Appendix IV.

II. THE DISCRETE MATERIAL MODEL

2.1. Description of the Undislocated Lattice

The discrete model of the crystal lattice will consist of a simple cubic arrangement of atoms for which the crystal boundaries will be parallel to the cubic axes. The atomic spacing is b and the x and y dimensions of the lattice are mb and nb respectively. Since the eventual problem involves only plane deformations, the z dimension is redundant.

Suppose that this lattice is in its minimum potential energy position as shown in Figure 3 and that in this position all atomic forces are zero. Now suppose that, in response to some arbitrary internal or external disturbance, the lattice undergoes a small plane deformation from its minimum potential configuration. What relationships exist between the displacement of the lattice point (i,j) and the displacements of all other lattice points in the crystal? The answer to this question depends on the form of the atomic bond forces between atom (i,j) and all other atoms in the system. These bond forces will be approximated in the following way: (1) the displacement of each lattice point is affected directly by its nearest and next nearest neighbors, (2) the relative

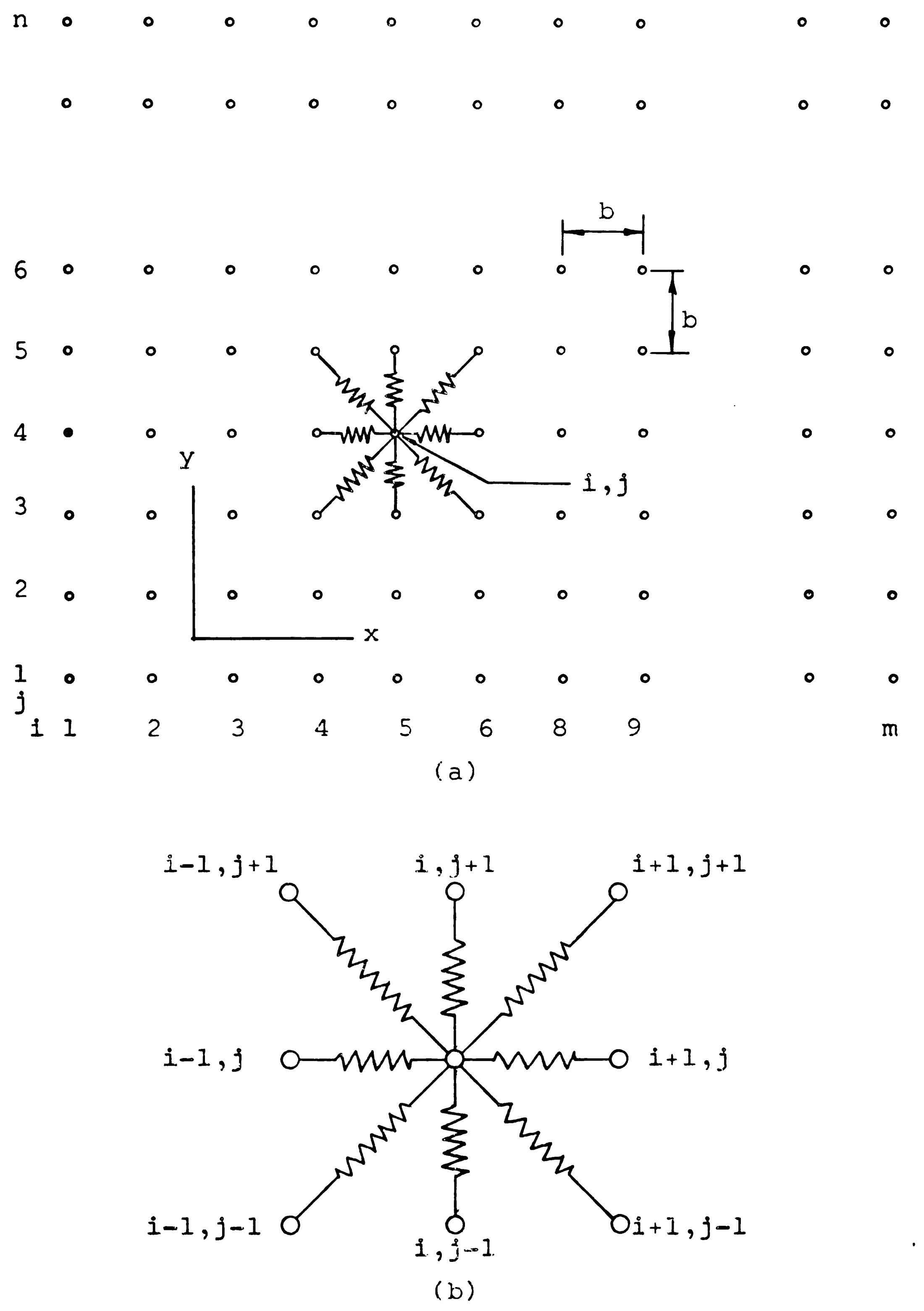


Fig. 3.--Simple cubic lattice in the undisturbed configuration with detail of lattice point i,j and its neighbors

displacement of two adjacent lattice points results in a restoring force which is linearly proportional to the displacement, and (3) the restoring force is directed along the line joining the two lattice points.

With these bond force characteristics the crystal may be visualized as an array of points each of which is connected to its nearest and next nearest neighbors by a linear spring. In the absence of a disturbance all the springs are unstretched. If the lattice is subjected to a plane disturbance, each lattice point is displaced to a new position. The mutual force between that atom at (i,j) and its nearest neighbor at point (i+1,j) is proportional to the length d = r-b in Figure 4a where d is given by the equation

$$d = r-b = [(b + u_{i+1,j} - u_{i,j})^2 + (v_{i+1,j} - v_{i,j})^2]^{1/2} - b. \qquad (2.1)$$

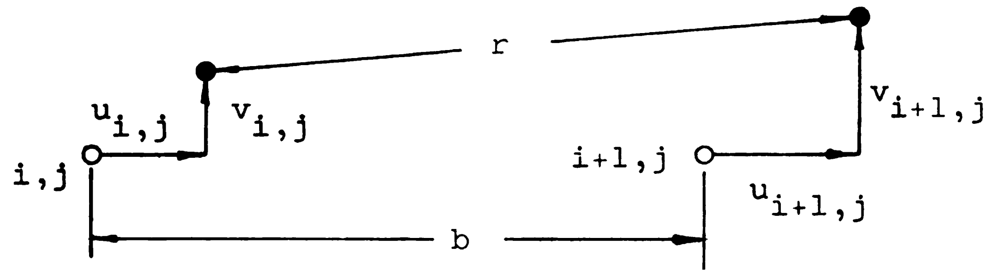
If the quantity $(v_{i+1,j} - v_{i,j})$ is small enough so that its square may be neglected, the length d in linearized form is given by

$$d = (u_{i+1,j} - u_{i,j}). \qquad (2.2)$$

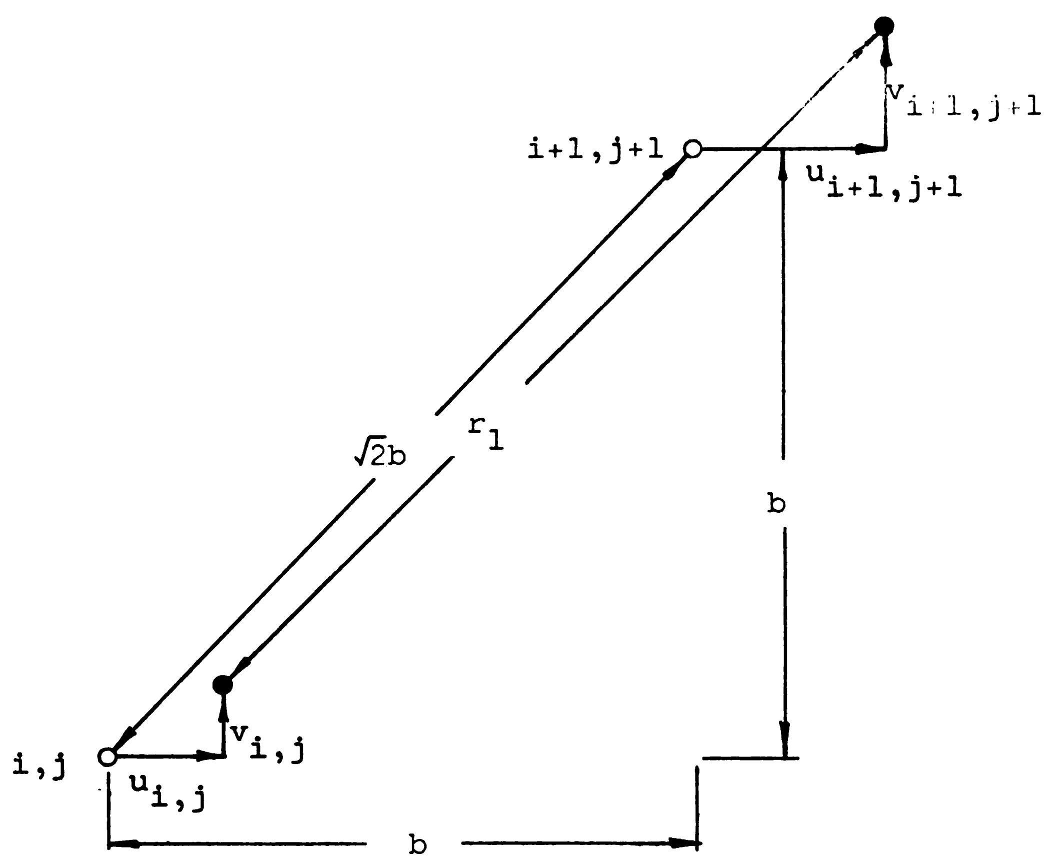
Assuming a force constant α, the force acting on the atom (i,j) is

$$F_{i,j} = \alpha(u_{i+1,j} - u_{i,j}). \qquad (2.3)$$

By virtue of the assumption that $(v_{i+1,j} - v_{i,j})$ is small compared to $\left[b + (u_{i+1,j} - u_{i,j})\right]$, the rotation of the bond force may be neglected so that the x and y components of



(a) Nearest Neighbors



(b) Next Nearest Neighbors

Fig. 4.--Neighboring lattice points in a displaced position

force acting on atom (i,j) due to its interaction with atom $(i+1,j)$ are

$$F_x = \alpha(u_{i+1,j} - u_{i,j})$$
$$F_y = 0. \qquad (2.4)$$

In a similar manner the force between atom (i,j) and its next nearest neighbor at $(i+1,j+1)$ is proportional to the distance $d_1 = r_1 - \sqrt{2}\, b$. Referring to Figure 4b

$$d_1 = r_1 - \sqrt{2}\, b = [(b + u_{i+1,j+1} - u_{i,j})^2 + (b + v_{i+1,j+1} - v_{i,j})^2]^{1/2} - \sqrt{2}\, b. \qquad (2.5)$$

Neglecting the terms involving $(u_{i+1,j+1} - u_{i,j})^2$ and $(v_{i+1,j+1} - v_{i,j})^2$ gives

$$d_1 = [2b^2 + 2b(u_{i+1,j+1} - u_{i,j} + v_{i+1,j+1} - v_{i,j})]^{1/2} - \sqrt{2}\, b. \qquad (2.6)$$

Expanding equation (2.6) in a binomial series gives

$$d_1 = \frac{1}{\sqrt{2}}[(u_{i+1,j+1} - u_{i,j}) + (v_{i+1,j+1} - v_{i,j})]. \qquad (2.7)$$

If the force constant is β, the mutual force on these two atoms is

$$F = \frac{\beta}{\sqrt{2}}[(u_{i+1,j+1} - u_{i,j}) + (v_{i+1,j+1} - v_{i,j})]. \qquad (2.8)$$

Neglecting the bond rotation, the force components on atom (i,j) due to its interaction with atom $(i+1,j+1)$ are

$$F_x = F_y = \frac{\beta}{2}[(u_{i+1,j+1} - u_{i,j}) + (v_{i+1,j+1} - v_{i,j})]. \qquad (2.9)$$

In the case of static equilibrium all such force interactions between atom (i,j) and its neighbors as shown in Figure 3b must produce a zero resultant. The equilibrium equations for atom (i,j) are

$$\sum F_x = 0$$

$$\alpha(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) + \frac{\beta}{2}(u_{i+1,j+1} + v_{i+1,j+1} + u_{i+1,j-1} - v_{i+1,j-1} + u_{i-1,j+1} - v_{i-1,j+1} + u_{i-1,j-1} + v_{i-1,j-1} - 4u_{i,j}) = 0 \quad (2.10)$$

$$\sum F_y = 0$$

$$\alpha(v_{i,j+1} - 2v_{i,j} + v_{i,j-1}) + \frac{\beta}{2}(u_{i+1,j+1} + v_{i+1,j-1} - u_{i+1,j-1} + v_{i+1,j-1} - u_{i-1,j+1} + v_{i-1,j+1} + u_{i-1,j-1} + v_{i-1,j-1} - 4v_{i,j}) = 0. \quad (2.11)$$

These equations are similar to those presented for a more general case by Kittel [10]. The equilibrium equation for lattice points on the boundary of the crystal are similar to equations (2.10) and (2.11) except that the effects of the missing neighbors are omitted. A lattice point on the lower boundary at point (i,1) has for example the equilibrium equations

$$\sum F_x = 0$$

$$\alpha(u_{i+1,1} - 2u_{i,1} + u_{i-1,1}) + \frac{\beta}{2}(u_{i+1,2} + v_{i+1,2} + u_{i-1,2} - v_{i-1,2} - 2u_{i,1}) = 0 \quad (2.12)$$

$$\sum F_y = 0$$

$$\alpha(v_{i,2} - v_{i,1}) + \frac{\beta}{2}(u_{i+1,2} + v_{i+1,2} - u_{i-1,2} + v_{i-1,2} - 2v_{i,1}) = 0. \quad (2.13)$$

These equations assume no external force acts on the lattice point.

2.2. Introduction of an Edge Dislocation into the Undisturbed Lattice

An edge dislocation will now be introduced into the initially undisturbed lattice shown in Figure 3a. At the lower boundary of the crystal between lattice point (r,1) and the succeeding point the atomic bonds, i.e., the linear springs, are severed up to a height $j = s$. A new plane of atoms, s atomic spacings high, is inserted into the gap resulting from this process. While the lattice is constrained in its undisturbed position, atomic bonds are established between atoms on the extra plane and their neighbors.

These bonds possess a high potential energy, i.e., the linear springs connecting the atoms on the extra plane with their neighbors are compressed, while the potential energy elsewhere remains zero because of the constraint of the lattice. The lattice constraint is now released and the potential energy concentration around the extra atom place is distributed through the lattice, resulting in the displacement of each lattice point from its original position. The force bonds between atoms on

the extra atom plane and its neighbors are shown in Figure 5. According to the sign convention given by Cottrell [2], this extra atom plane produces a negative edge dislocation in the crystal lattice.

2.3. Bond Forces on the Extra Atom Plane

The most important factor in determining the lattice deformation is the form of the interatomic forces between atoms on the extra plane and their neighbors. These forces will now be discussed in detail.

Consider a lattice point $(r+1,j)$ on the extra atom plane and its nearest neighbor at point (r,j). When the lattice is in the constrained position, these points are separated by half an atomic spacing, $.5b$. Assume that the mutual bond force is zero when the separation is the normal atomic spacing b and that the mutual atomic force is linearly related to the difference between the zero force separation and the actual separation. In the constrained position then, there is mutual repulsive force of $.5b\alpha$ on atoms $(r+1,j)$ and (r,j) where the force constant is assumed to be the same as that for normal nearest neighbor interactions. Upon removal of the constraints the points $(r+1,j)$ and (r,j) will move to their displaced positions as shown in Figure 6a. The difference between the displaced separation of these two points and the assumed zero force separation is

$$d_2 = b - [(.5b + u_{r+1,j} - u_{r,j})^2 + (v_{r+1,j} - v_{r,j})^2]^{1/2}. \tag{2.14}$$

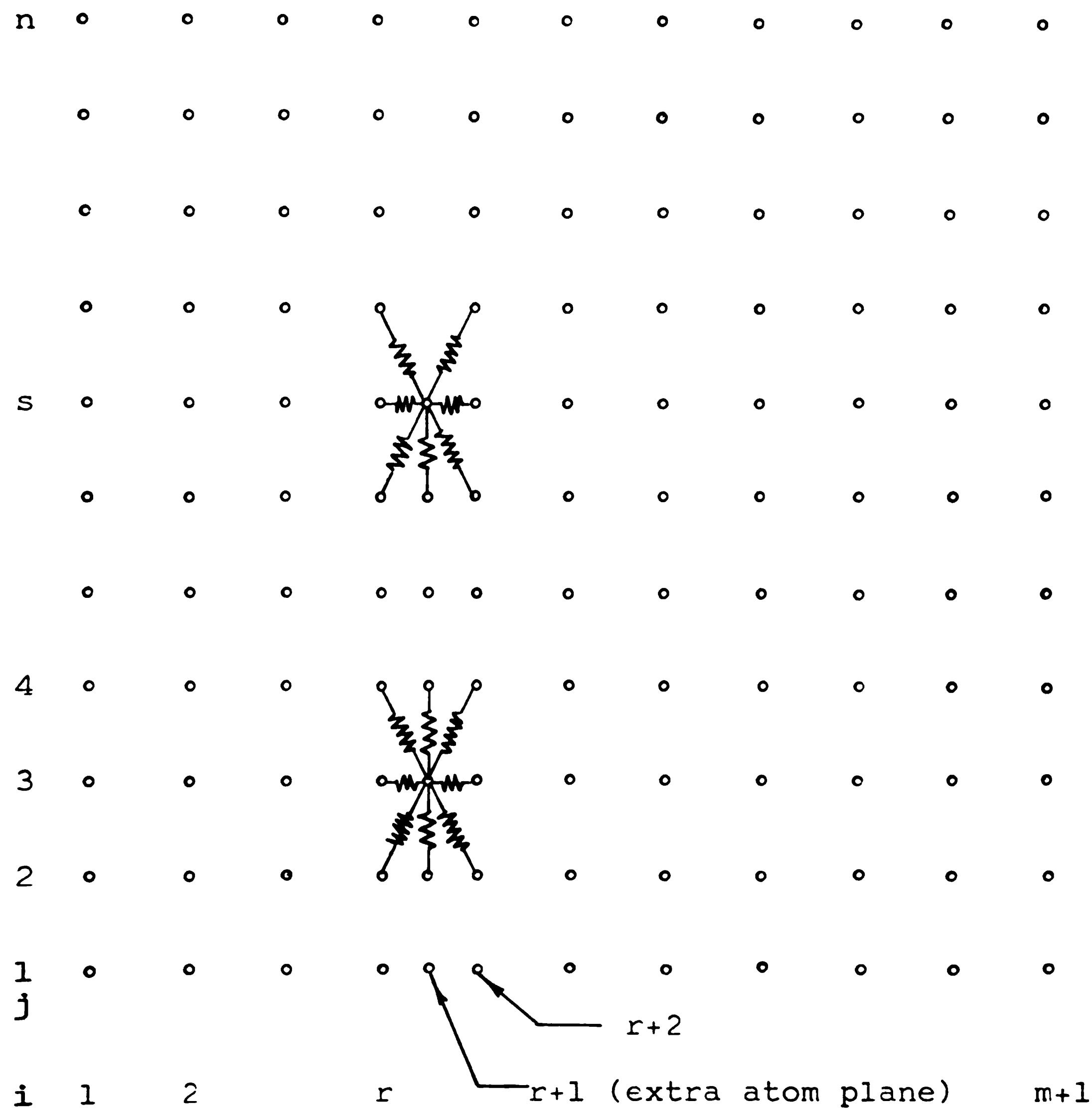


Fig. 5.--Constrained lattice after the addition of the extra atom plane

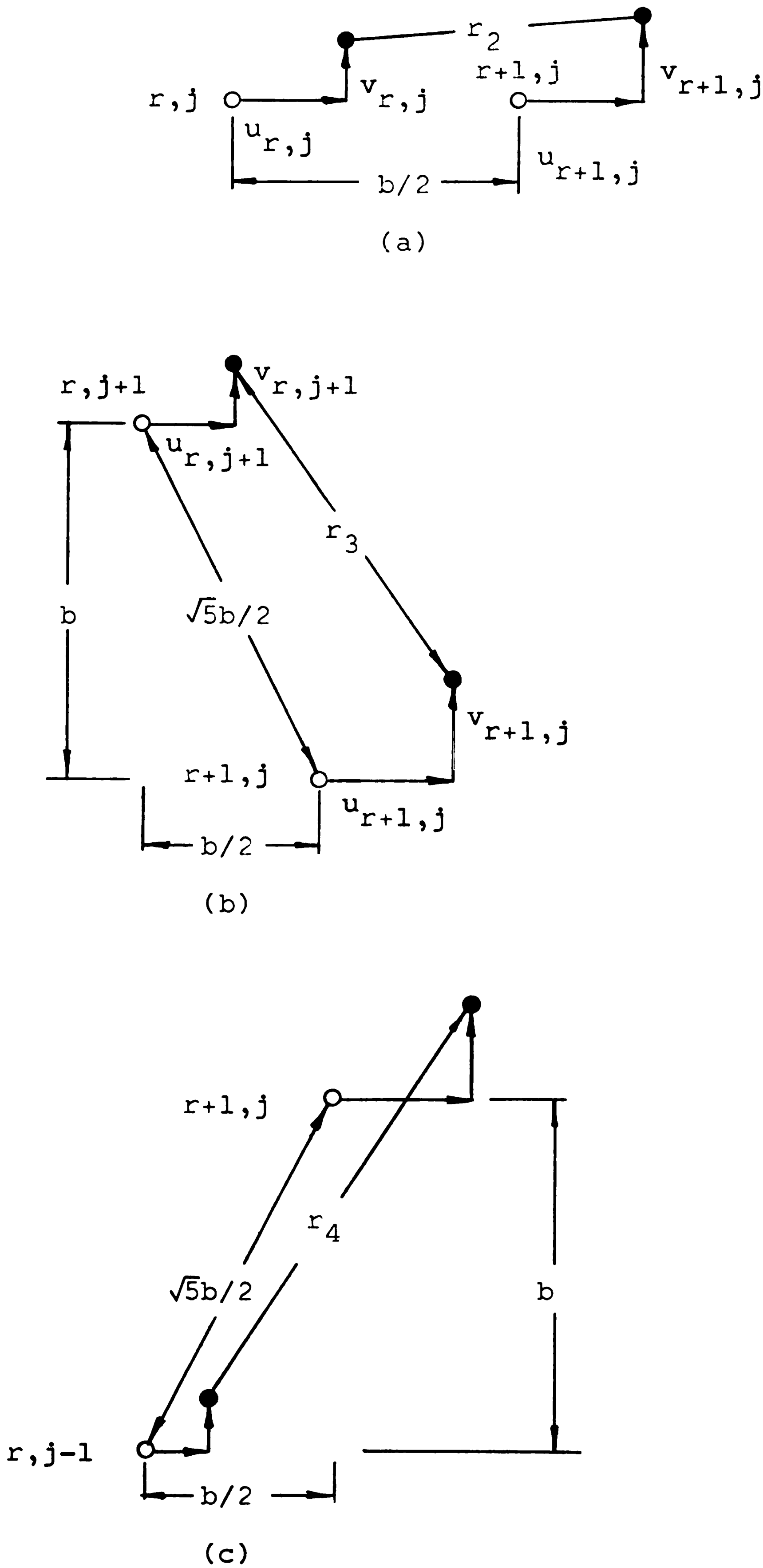


Fig. 6.--Neighboring lattice points on extra atom plane

Neglecting the quantity $(v_{r+1,j} - v_{r,j})^2$ as small compared with other terms in the bracket gives

$$d_2 = b - [.5b + (u_{r+1,j} - u_{r,j})] \tag{2.15}$$

$$d_2 = .5b + (u_{r,j} - u_{r+1,j}). \tag{2.16}$$

Assuming a linear relation between d_2 and the bond force results in a mutual repulsive force acting on atoms (r+1,j) and (r,j) of magnitude

$$.5b\alpha + \alpha(u_{r,j} - u_{r+1,j}). \tag{2.17}$$

If the rotation of the bond is small, and this seems to be a reasonable assumption for the atom pairs of which this is a typical example, the components of force on atom (r+1,j) are

$$\begin{aligned} F_x &= .5b\alpha + \alpha(u_{r,j} - u_{r+1,j}) \\ F_y &= 0. \end{aligned} \tag{2.18}$$

The interaction between the atom (r+1,j) and its next nearest neighbor at (r,j+1) may be similarly determined. In the constrained position of the lattice these atoms are separated by the distance $\frac{\sqrt{5}}{2}b$. If it is assumed that the zero force separation for all next nearest neighbors is $\sqrt{2}\,b$ and that a linear relationship exists between atomic force and the difference between actual separation and zero force separation, then a mutual repulsive force of $\beta(\sqrt{2}\,b - \frac{\sqrt{5}}{2}b)$ acts on atoms (r+1,j) and (r,j+1) when the lattice is in the constrained position. After relaxing the constraints the difference between actual and zero force separation is seen from Figure 6b to become

$$d_3 = \sqrt{2}\,b - p_2 = \sqrt{2}\,b - [(.5b + u_{r+1,j} - u_{r,j+1})^2 + (b + v_{r,j+1} - v_{r+1,j})^2]^{1/2}. \tag{2.19}$$

Neglecting orders of $(u_{r+1,j} - u_{r,j+1})$ and $(v_{r,j+1} - v_{r+1,j})$ of two and higher leaves the linearized form

$$d_3 = \sqrt{2}\,b - [\frac{\sqrt{5}}{2}b + \frac{1}{\sqrt{5}}(u_{r+1,j} - u_{r,j+1}) + \frac{2}{\sqrt{5}}(v_{r,j+1} - v_{r+1,j})]. \tag{2.20}$$

Assuming a linear relationship between the atomic force and d_3 results in a mutual repulsive force on atoms (r+1,j) and (r,j+1) of

$$F = (\sqrt{2} - \frac{\sqrt{5}}{2})b\beta - \frac{\beta}{\sqrt{5}}(u_{r+1,j} - u_{r,j+1}) - \frac{2\beta}{\sqrt{5}}(v_{r,j+1} - v_{r+1,j}). \tag{2.21}$$

It will be initially assumed that the bond rotation between atom pairs of this type may be neglected. This assumption, however, for this particular type of atom pair may not be justified. Whether some different bond orientation should be used will be determined after the displacement solution of a particular numerical example has been found and examined. In any case, according to the initial assumption, the x and y force components on atom (r+1,j) are

$$F_x = \frac{F}{\sqrt{5}} = \left(\sqrt{\frac{2}{5}} - \frac{1}{2}\right)b\beta - \frac{\beta}{5}(u_{r+1,j} - u_{r,j+1}) -$$

$$\frac{2\beta}{5}(v_{r,j+1} - v_{r+1,j}) \qquad (2.22)$$

$$F_y = -\frac{2F}{\sqrt{5}} = -2\left(\sqrt{\frac{2}{5}} - \frac{1}{2}\right)b\beta + \frac{2\beta}{5}(u_{r+1,j} - u_{r,j+1}) +$$

$$\frac{4\beta}{5}(v_{r,j+1} - v_{r+1,j}).$$

The force components on atom (r+1,j) due to its interaction with atom (r,j-1) which are shown in Figure 6c are

$$F_x = \left(\sqrt{\frac{2}{5}} - \frac{1}{2}\right)b\beta + \frac{\beta}{5}(u_{r,j-1} - u_{r+1,j}) + \frac{2\beta}{5}(v_{r,j-1} - v_{r+1,j})$$

$$F_y = 2\left(\sqrt{\frac{2}{5}} - \frac{1}{2}\right)b\beta + \frac{2\beta}{5}(u_{r,j-1} - u_{r+1,j}) + \frac{4\beta}{5}(v_{r,j-1} - v_{r+1,j}). \qquad (2.23)$$

The assumptions involved in defining the bond forces in this way are formidable. The linearity between force and displacement up to a relative displacement of half an atomic spacing is the most unrealistic of all assumptions. The simplification in calculations which results from such an idealization is, of course, the justifying factor. The neglect of second powers of the relative displacements is a good approximation up to values of relative displacement of about .3b which may be seen from Figure 7. The neglect of bond rotation is certainly reasonable up to angles of five or six degrees and the values of displacement involved in any foreseeable application of this theory should be such that most bond rotations are within this limit. A correction can be applied to any bond rotations which exceed the limiting value.

$$\frac{F}{\beta} = \sqrt{2}b - \left[\frac{\sqrt{5}b}{2} + b + b(u_r + 2u_r) + u_r^{\,2} + v_r^{\,2}\right]^{1/2}$$

$$\frac{F}{\beta} \simeq \sqrt{2}b - \left[\frac{\sqrt{5}b}{2} - \frac{1}{\sqrt{5}}(u_r + 2v_r)\right] \quad \text{(linearized)}$$

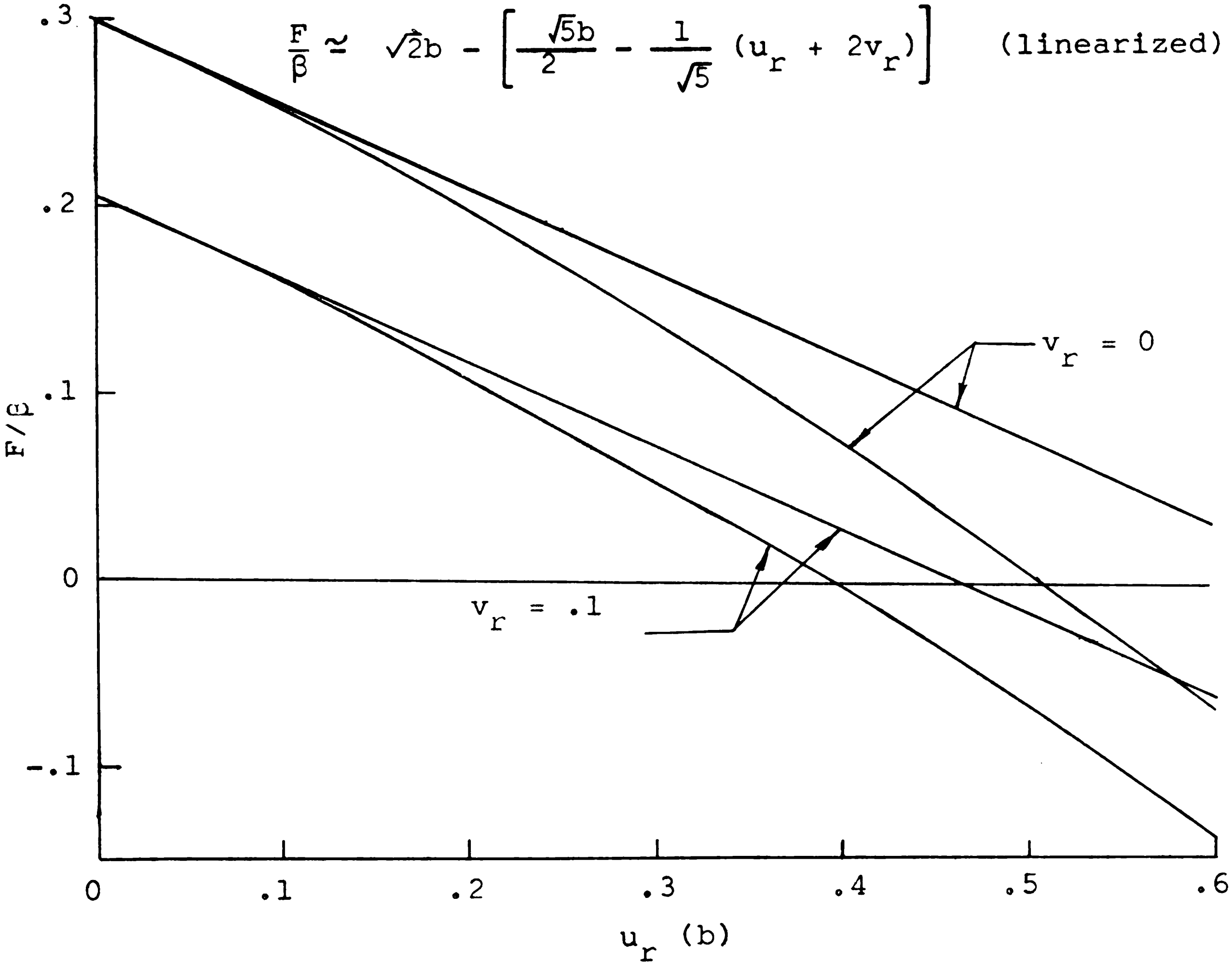


Fig. 7.--F/β versus relative u for constant relative v

Despite the formidable assumptions which must be made to facilitate a solution, this model does possess, in a simple way, the discrete character of a real crystal lattice and is superior to the ordinary continuum model in this regard.

2.4. Equilibrium Equations for Lattice Points in the Crystal

The equilibrium equations for those atoms which are surrounded by a normal complement of nearest and next nearest neighbors and do not lie on or next to the extra atom plane are given by the equations (2.10) and (2.11). Referring to Figure 5a all lattice points for which i and j satisfy the relationships

$$2 \leq i \leq m$$

$$2 \leq j \leq n-1$$

where

$$i \neq r,\ r+1, r+2 \text{ for } j \leq s+1$$

have equations (2.10) and (2.11) as equilibrium equations. All lattice points on the lower boundary except at the corners and on or next to the extra atom plane, that is, points for which i and j satisfy the relations

$$2 \leq i \leq m \qquad i \neq r,\ r+1, r+2$$

$$j = 1,$$

have equations (2.12) and (2.13) as equilibrium equations.

The equilibrium for all other lattice points will now be listed along with the appropriate values of the indices i and j.

a) At the lower left-hand corner of the crystal

$i = 1$

$j = 1$

$$\sum F_x = 0 \qquad \alpha(u_{2,1} - u_{1,1}) + \frac{\beta}{2}(u_{2,2} + v_{2,2} - u_{1,1} - v_{1,1}) = 0 \qquad (2.24)$$

$$\sum F_y = 0 \qquad \alpha(v_{1,2} - v_{1,1}) + \frac{\beta}{2}(u_{2,2} + v_{2,2} - u_{1,1} - v_{1,1}) = 0. \qquad (2.25)$$

b) For the left-hand boundary

$i = 1$

$2 \leq j \leq n-1$

$$\sum F_x = 0 \qquad \alpha(u_{2,j} - u_{1,j}) + \frac{\beta}{2}(u_{2,j+1} + v_{2,j+1} + u_{2,j-1} - v_{2,j-1} - 2u_{1,j}) = 0 \qquad (2.26)$$

$$\sum F_y = 0 \qquad \alpha(v_{1,j+1} - 2v_{1,j} + v_{1,j-1}) + \frac{\beta}{2}(u_{2,j+1} + v_{2,j+1} - u_{2,j-1} + v_{2,j-1} - 2u_{1,j}) = 0. \qquad (2.27)$$

c) At upper left-hand boundary

$i = 1$

$j = n$

$$\sum F_x = 0 \qquad \alpha(u_{2,n} - u_{1,n}) + \frac{\beta}{2}(u_{2,n-1} - v_{2,n-1} - u_{1,n} + v_{1,n}) = 0 \qquad (2.28)$$

$$\sum F_y = 0 \qquad \alpha(v_{1,n-1} - v_{1,n}) + \frac{\beta}{2}(-u_{2,n-1} + v_{2,n-1} + u_{1,n} - v_{1,n}) = 0. \qquad (2.29)$$

d) For the upper boundary noting that there is no lattice plane for $i = r+1$ so that i skips directly from $i = r$ to $i = r+2$

$$2 \leq i \leq m \qquad i \neq r,\ r+1,\ r+2$$

$$j = n$$

$$\sum F_x = 0 \qquad \alpha(u_{i+1,n} - u_{i,n} + u_{i-1,n}) + \frac{\beta}{2}(u_{i+1,n-1} - v_{i+1,n-1} + u_{i-1,n-1} + v_{i-1,n-1} - 2u_{i,n}) = 0 \tag{2.30}$$

$$\sum F_y = 0 \qquad \alpha(v_{i,n-1} - v_{i,n}) + \frac{\beta}{2}(-u_{i+1,n-1} + v_{i+1,n-1} + u_{i-1,n-1} + v_{i-1,n-1} - 2v_{i,n}) = 0. \tag{2.31}$$

e) For the point

$$i = r$$

$$j = n$$

$$\sum F_x = 0 \qquad \alpha(u_{r+2,n} - 2u_{r,n} + u_{r-1,n}) + \frac{\beta}{2}(u_{r+2,n-1} - v_{r+2,n-1} + u_{r-1,n-1} + v_{r-1,n-1} - 2u_{r,n}) = 0 \tag{2.32}$$

$$\sum F_y = 0 \qquad \alpha(v_{r,n-1} - v_{r,n}) + \frac{\beta}{2}(-u_{r+2,n-1} + v_{r+2,n-1} + u_{r-1,n-1} + v_{r-1,n-1} - 2v_{r,n}) = 0. \tag{2.33}$$

f) For points on the plane to the left of the extra atom plane which lie above the extra atom plane

$$i = r$$

$$n-1 \geq j \geq s+2$$

$$\sum F_x = 0 \qquad \alpha(u_{r+2,j} - 2u_{r,j} + u_{r-1,j}) + \frac{\beta}{2}(u_{r+2,j+1} + v_{r+2,j+1} + u_{r+2,j-1} - v_{r+2,j-1} + u_{r-1,j-1} + v_{r-1,j-1} + u_{r-1,j+1} - v_{r-1,j-1} - 4u_{r,j}) = 0 \tag{2.34}$$

$$\sum F_y = 0 \qquad \alpha(v_{r,j+1} - 2v_{r,j} + v_{r,j-1}) + \frac{\beta}{2}(u_{r+2,j+1} + v_{r+2,j+1} - u_{r+2,j-1} + v_{r+2,j-1} + u_{r-1,j-1} + v_{r-1,j-1} - u_{r-1,j+1} + v_{r-1,j-1} + 4v_{r,j}) = 0. \tag{2.35}$$

g) For the lattice point at

$i = r$

$j = s+1$

whose bonds are shown in Figure 8a

$$\sum F_x = 0 \qquad \alpha(u_{r+2,s+1} - 2u_{r,s+1} + u_{r-1,s+1}) + \frac{\beta}{2}(u_{r+2,s+2} + v_{r+2,s+2} + u_{r-1,s} + v_{r-1,s} + u_{r-1,s+2} - v_{r-1,s+2} + u_{r+2,s} - v_{r+2,s} - 4u_{r,s+1}) - .13246b\beta + \frac{\beta}{5}(u_{r+1,s} - u_{r,s+1}) + \frac{2\beta}{5}(v_{r,s+1} - v_{r+1,s}) = 0 \tag{2.36}$$

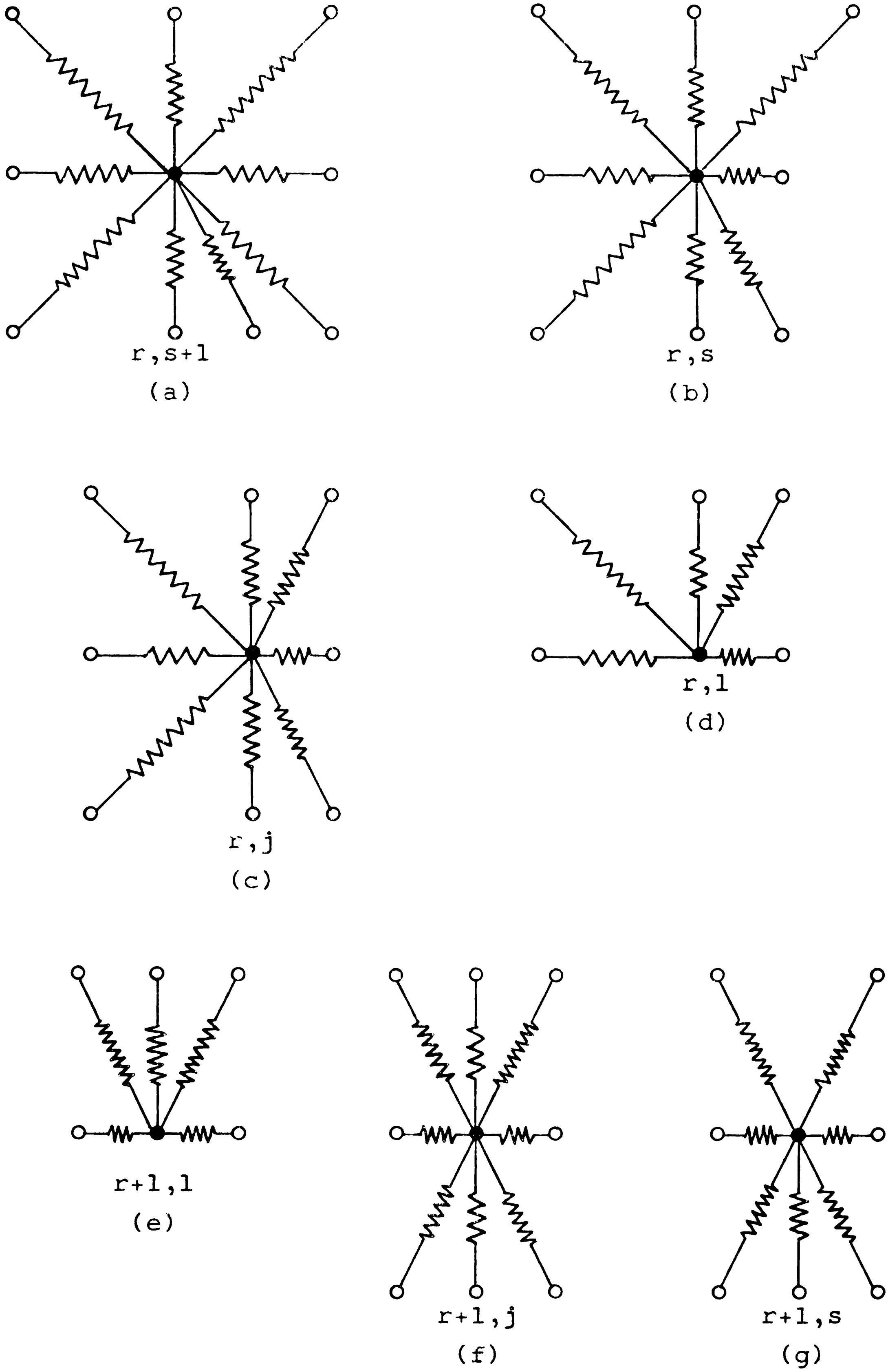


Fig. 8.--Force bonds for lattice points on and to the left of the extra atom plane

$$\sum F_y = 0 \qquad \alpha(v_{r,s+2} - 2v_{r,s+1} + v_{r,s}) + \frac{\beta}{2}(u_{r+2,s+2} + v_{r+2,s+2} - u_{r+2,s} + v_{r+2,s} + u_{r-1,s} + v_{r-1,s} - u_{r-1,s+2} + v_{r-1,s+2} - 4v_{r,s+1}) + .26492b\beta - \frac{2\beta}{5}(u_{r+1,s} - u_{r,s+1}) - \frac{4\beta}{5}(v_{r,s+1} - v_{r+1,s}) = 0. \tag{2.37}$$

h) For the lattice point at

$i = r$

$j = s$

whose bonds are shown in Figure 8b the equilibrium equations are

$$\sum F_x = 0 \qquad \alpha(-.5b + u_{r+1,s} - 2u_{r,s} + u_{r-1,s}) + \frac{\beta}{2}(u_{r+2,s+1} + v_{r+2,s+1} + u_{r-1,s-1} + v_{r-1,s-1} + u_{r-1,s+1} - v_{r-1,s+1} - v_{r,s} - 3u_{r,s}) - .13246b\beta + \frac{\beta}{5}(u_{r+1,s-1} - u_{r,s}) + \frac{2\beta}{5}(v_{r,s} - v_{r+1,s-1}) = 0 \tag{2.38}$$

$$\sum F_y = 0 \qquad \alpha(v_{r,s+1} - 2v_{r,s} + v_{r,s-1}) + \frac{\beta}{2}(u_{r+2,s+1} + v_{r+2,s+1} + u_{r-1,s-1} + v_{r-1,s-1} - u_{r-1,s+1} + v_{r-1,s+1} - u_{r,s} - 3v_{r,s}) + .26492b\beta - \frac{2\beta}{5}(u_{r+1,s-1} - u_{r,s}) + \frac{2\beta}{5}(v_{r,s} - v_{r+1,s-1}) = 0. \tag{2.39}$$

i) The equilibrium equations for lattice point

$i = r$

$s-1 \geq j \geq 2$

referring to Figure 8c are

$$\sum F_x = 0 \qquad \alpha(-.5b + u_{r+1,j} - 2u_{r,j} + u_{r-1,j}) + \frac{\beta}{2}(u_{r-1,j+1} - v_{r-1,j+1} + u_{r-1,j-1} + v_{r-1,j-1} - 2u_{r,j}) - .26492b\beta + \frac{\beta}{5}(u_{r+1,j+1} - u_{r,j}) + \frac{2\beta}{5}(v_{r+1,j+1} - v_{r,j}) - \frac{\beta}{5}(u_{r+1,j-1} - u_{r,j}) - \frac{2\beta}{5}(v_{r,j} - v_{r+1,j-1}) = 0 \qquad (2.40)$$

$$\sum F_y = 0 \qquad \alpha(v_{r,j+1} - 2v_{r,j} + v_{r,j-1}) + \frac{\beta}{2}(u_{r-1,j-1} + v_{r-1,j-1} + u_{r-1,j+1} - v_{r-1,j+1} - 2v_{r,j}) + \frac{2\beta}{5}(u_{r+1,j+1} - u_{r,j}) + \frac{4\beta}{5}(v_{r+1,j+1} - v_{r,j}) - \frac{2\beta}{5}(u_{r+1,j-1} - u_{r,j}) - \frac{4\beta}{5}(v_{r,j} - v_{r+1,j-1}) = 0. \qquad (2.41)$$

j) With reference to Figure 8d the equilibrium equations for lattice point

$i = r$

$j = 1$

are

$$\sum F_x = 0 \qquad \alpha(-.5b + u_{r+1,1} - 2u_{r,1} + u_{r-1,1}) + \frac{\beta}{2}(u_{r-1,2} - u_{r,1} - v_{r-1,2} + v_{r,1}) - .13246b\beta + \frac{\beta}{2}(u_{r+1,2} - u_{r,1}) + \frac{2\beta}{5}(v_{r+1,2} - v_{r,1}) = 0. \tag{2.42}$$

$$\sum F_y = 0 \qquad \alpha(v_{r,2} - v_{r,1}) + \frac{\beta}{2}(-u_{r-1,2} + u_{r,1} + v_{r-1,2} - v_{r,1}) - .26492\beta b + \frac{2\beta}{5}(u_{r+1,2} - u_{r,1}) + \frac{4\beta}{5}(v_{r+1,2} - v_{r,1}) = 0. \tag{2.43}$$

k) The equilibrium equations for point

$i = r+1$

$j = 1$

whose bonds are shown in Figure 8e are

$$\sum F_x = 0 \qquad \alpha(u_{r,1} - 2u_{r+1,1} + u_{r+2,1}) + \frac{\beta}{5}(u_{r,2} - u_{r+1,1}) + \frac{2\beta}{5}(v_{r+1,1} - v_{r,2}) + \frac{\beta}{5}(u_{r+2,2} - u_{r+1,1}) + \frac{2\beta}{5}(v_{r+2,2} - v_{r+1,1}) = 0 \tag{2.44}$$

$$\sum F_y = 0 \qquad \alpha(v_{r+1,2} - v_{r+1,1}) - .26492b\beta + \frac{2\beta}{5}(u_{r,2} - u_{r+1,1}) + \frac{4\beta}{5}(v_{r+1,1} - v_{r,2}) - .26492b\beta + \frac{2\beta}{5}(u_{r+2,2} - u_{r+1,1}) + \frac{4\beta}{5}(v_{r+2,2} - v_{r+1,1}) = 0. \tag{2.45}$$

l) The equilibrium equations for

$i = r+1$

$2 \leq j \leq s-1$

shown in Figure 8f are

$$\sum F_x = 0 \qquad \alpha(u_{r,j} - 2u_{r+1,j} + u_{r+2,j}) + \frac{\beta}{5}(u_{r+2,j+1} + u_{r,j-1} + u_{r,j+1} + u_{r+2,j-1} - 4u_{r+1,j}) + \frac{2\beta}{5}(v_{r+2,j+1} + v_{r,j-1} - v_{r,j+1} - v_{r+2,j-1}) = 0 \tag{2.46}$$

$$\sum F_y = 0 \qquad \alpha(v_{r+1,j+1} - 2v_{r+1,j} + v_{r+1,j-1}) + \frac{2\beta}{5}(u_{r+2,j+1} + u_{r,j-1} - u_{r,j+1} - u_{r+2,j-1}) + \frac{4\beta}{5}(v_{r+2,j+1} + v_{r,j-1} + v_{r,j+1} + v_{r+2,j-1} - 4v_{r+1,j}) = 0. \tag{2.47}$$

m) At the point

$i = r+1$

$j = s$

with bonds shown in the Figure 8g the equilibrium equations are

$$\sum F_x = 0 \qquad \alpha(u_{r,s} - 2u_{r+1,s} + u_{r+2,s}) + \frac{\beta}{5}(u_{r+2,s+1} + u_{r,s-1} + u_{r+2,s-1} + u_{r,s+1} - 4u_{r+1,s}) + \frac{2\beta}{5}(v_{r+2,s+1} + v_{r,s-1} - v_{r+2,s-1} - v_{r,s+1}) = 0 \tag{2.48}$$

$$\sum F_y = 0 \qquad \alpha(v_{r+1,s-1} - v_{r+1,s}) + \frac{2\beta}{5}(u_{r+2,s+1} + u_{r,s-1} - u_{r,s+1} - u_{r+2,s-1}) + \frac{4\beta}{5}(v_{r+2,s+1} + v_{r,s-1} + v_{r,s+1} + v_{r+2,s-1} - 4v_{r+1,s}) = 0. \tag{2.49}$$

n) At the lattice point

$i = r+2$

$j = n$

$$\sum F_x = 0 \qquad \alpha(u_{r+3,n} - 2u_{r+2,n} + u_{r,n}) + \frac{\beta}{2}(u_{r,n-1} + v_{r,n-1} + u_{r+3,n-1} - v_{r+3,n-1} - 2u_{r+2,n}) = 0$$

$$\sum F_y = 0 \qquad \alpha(v_{r+2,n-1} - v_{r+2,n}) + \frac{\beta}{2}(u_{r,n-1} + v_{r,n-1} - u_{r+3,n-1} + v_{r+3,n-1} - 2v_{r+2,n}) = 0.$$

o) For lattice points on the plane to the right of and above the extra plane where

$i = r+2$

$n-1 \geq j \geq s+2$

$$\sum F_x = 0 \qquad \alpha(u_{r+3,j} - 2u_{r+2,j} + u_{r,j}) + \frac{\beta}{2}(u_{r+3,j+1} + u_{r,j+1} + v_{r+3,j+1} - v_{r,j+1} + u_{r,j-1} + v_{r,j-1} - u_{r+3,j-1} + v_{r+3,j-1} - 4u_{r+2,j}) = 0$$

$$\sum F_y = 0 \qquad \alpha(v_{r+2,j+1} - 2v_{r+2,j} + v_{r+2,j-1}) + \frac{\beta}{2}(u_{r+3,j+1} - u_{r,j+1} + v_{r+3,j+1} + v_{r,j+1} + u_{r,j-1} + v_{r,j-1} - u_{r+3,j-1} + v_{r+3,j-1} - 4v_{r+2,j}) = 0.$$

p) For the lattice point at

$i = r+2$

$j = s+1$

$$\sum F_x = 0 \qquad \alpha(u_{r,s+1} - 2u_{r+2,s+1} + u_{r+3,s+1}) +$$

$$\frac{\beta}{2}(u_{r+3,s+2} + u_{r,s+2} + v_{r+3,s+2} - v_{r,s+2} +$$

$$u_{r,s} + v_{r,s} - u_{r+3,s} + v_{r+3,s} - 4v_{r+2,s+1}) +$$

$$.13246b\beta - \frac{\beta}{5}(u_{r+2,s+1} - u_{r+1,s}) -$$

$$\frac{2\beta}{5}(v_{r+2,s+1} - v_{r+1,s}) = 0$$

$$\sum F_y = 0 \qquad \alpha(v_{r+2,s+2} - 2v_{r+2,s+1} + v_{r+2,s}) +$$

$$\frac{\beta}{2}(u_{r+3,s+2} - u_{r,s+2} + v_{r+3,s+2} + v_{r,s+2} +$$

$$u_{r,s} + v_{r,s} - u_{r+3,s} + v_{r+3,s} - 4v_{r+2,s+1}) +$$

$$.26492b\beta - \frac{2\beta}{5}(u_{r+2,s+1} - u_{r+1,s}) -$$

$$\frac{4}{5}(v_{r+2,s+1} - v_{r+1,s}) = 0.$$

q) At the lattice point

$i = r+2$

$j = s$

$$\sum F_x = 0 \qquad .5b\alpha + (u_{r+1,s} - 2u_{r+2,s} + u_{r+3,s}) +$$

$$\frac{\beta}{2}(u_{r+3,s+1} + v_{r+3,s+1} + u_{r,s+1} - v_{r,s+1} +$$

$$v_{r+2,s} + u_{r+3,s-1} - v_{r+3,s-1} - 3u_{r+2,s}) +$$

$$.13246b\beta - \frac{\beta}{5}(u_{r+2,s} - u_{r+1,s-1}) -$$

$$\frac{2\beta}{5}(v_{r+2,s} - v_{r+1,s-1}) = 0$$

$$\sum F_y = 0 \qquad \alpha(v_{r+2,s+1} - 2v_{r+2,s} + v_{r+2,s-1}) +$$

$$\frac{\beta}{2}(u_{r+3,s+1} + v_{r+3,s+1} - u_{r,s+1} + v_{r,s+1} -$$

$$u_{r+3,s-1} + u_{r+2,s} + v_{r+3,s-1} - 3v_{r+2,s}) +$$

$$.26492b\beta - \frac{2\beta}{5}(u_{r+2,s} - u_{r+1,s-1}) -$$

$$\frac{4\beta}{5}(v_{r+2,s} - v_{r+1,s-1}) = 0.$$

r) For lattice points

$i = r+2$

$2 \leq j \leq s-1$

$$\sum F_x = 0 \qquad .5b\alpha + \alpha(u_{r+1,j} - 2u_{r+2,j} + u_{r+3,j}) +$$

$$\frac{\beta}{2}(u_{r+3,j+1} + v_{r+3,j+1} + u_{r+3,j-1} - v_{r+3,j-1} -$$

$$2u_{r+2,j}) + .26492b\beta - \frac{\beta}{5}(u_{r+2,j} - u_{r+1,j-1}) -$$

$$\frac{2\beta}{5}(v_{r+2,j} - v_{r+1,j-1}) - \frac{\beta}{5}(u_{r+2,j} - u_{r+1,j+1}) -$$

$$\frac{2\beta}{5}(v_{r+1,j+1} - v_{r+2,j}) = 0$$

$$\sum F_y = 0 \qquad \alpha(v_{r+2,j+1} - 2v_{r+2,j} + v_{r+2,j-1}) +$$

$$\frac{\beta}{2}(u_{r+3,j+1} + v_{r+3,j+1} - u_{r+3,j-1} + v_{r+3,j-1} -$$

$$2v_{r+2,j}) + \frac{2\beta}{5}(u_{r+2,j} - u_{r+1,j-1}) + \frac{4\beta}{5}(v_{r+2,j} -$$

$$v_{r+1,j-1}) - \frac{2\beta}{5}(u_{r+2,j} - u_{r+1,j+1}) -$$

$$\frac{4\beta}{5}(v_{r+1,j+1} - v_{r+2,j}) = 0.$$

s) For the lattice point

$i = r+2$

$j = 1$

$$\sum F_x = 0 \qquad .5b\alpha + \alpha(u_{r+1,1} - 2u_{r+2,1} + u_{r+3,1}) + \frac{\beta}{2}(u_{r+3,2} - u_{r+2,1} + v_{r+3,2} - v_{r+2,1}) + .13246b\beta - \frac{\beta}{5}(u_{r+2,1} - u_{r+1,2}) - \frac{2\beta}{5}(v_{r+1,2} - v_{r+2,1}) = 0$$

$$\sum F_y = 0 \qquad \alpha(v_{r+2,2} - v_{r+2,1}) + \frac{\beta}{2}(u_{r+3,2} - u_{r+2,1} + v_{r+3,2} - v_{r+2,1}) - .26492b\beta + \frac{2\beta}{5}(u_{r+2,1} - u_{r+1,2}) - \frac{4\beta}{5}(v_{r+1,2} - v_{r+2,1}) = 0.$$

t) For the upper right hand corner where

$i = m$

$j = n$

$$\sum F_x = 0 \qquad \alpha(u_{m-1,n} - u_{m,n}) + \frac{\beta}{2}(u_{m-1,n-1} - u_{m,n} + v_{m-1,n-1} - v_{m,n}) = 0$$

$$\sum F_y = 0 \qquad \alpha(v_{m,n-1} - v_{m,n}) + \frac{\beta}{2}(u_{m-1,n-1} - u_{m,n} + v_{m-1,n-1} - v_{m,n}) = 0.$$

u) For lattice points on the right side boundary

$i = m$

$2 \leq j \leq n-1$

$$\sum F_x = 0 \qquad \alpha(u_{m-1,j} - u_{m,j}) + \frac{\beta}{2}(u_{m-1,j-1} + v_{m-1,j-1} + u_{m-1,j+1} - v_{m-1,j+1} - 2u_{m,j}) = 0$$

$$\sum F_y = 0 \qquad \alpha(v_{m,j+1} - 2v_{m,j} + v_{m,j-1}) + \frac{\beta}{2}(u_{m-1,j-1} + v_{m-1,j-1} - u_{m-1,j+1} + v_{m-1,j+1} - 2v_{m,j}) = 0.$$

v) For the lower right hand corner

$i = m$

$j = 1$

$$F_x = 0 \qquad \alpha(u_{m-1,1} - u_{m,1}) - \frac{\beta}{2}(u_{m,1} - u_{m-1,2} + v_{m-1,2} - v_{m,1}) = 0$$

$$F_y = 0 \qquad \alpha(v_{m,2} - v_{m,1}) + \frac{\beta}{2}(u_{m,1} - u_{m-1,2} + v_{m-1,2} - v_{m,1}) = 0.$$

These equations form a system of $2(mn + s)$ members for the $2(mn + s)$ unknown u and v displacements.

Because every term in the system of equilibrium equations originally was in the form of a difference between two x or two y displacements, $u_1 - u_2$ or $v_1 - v_2$, the solution is not unique. Given u and v displacements which satisfy the system of equilibrium equations, a new set of u's and v's formed by adding a constant quantity to the original u's and another constant quantity to the original v's will also satisfy the system of equations. This is physically reasonable since it must be possible to arbitrarily locate the crystal lattice in space. The lattice will be located by giving the x displacement of one lattice point and the y displacement of the same or of another lattice point arbitrary values. The x component of the equilibrium equation at the lattice point

where u is given and the y component of the equilibrium equation at the lattice point where v is given are then omitted from the system of equations. The resulting system of $2(mn + s) - 2$ equations may now be uniquely solved.

For purposes of this dissertation the preceding system of equations will be solved for the specific case of a dislocation which is symmetrically located in a square crystal. The geometric parameters of Figure 5a will be given the values

$$n = 33$$
$$m = 34$$
$$r = 17$$
$$s = 17.$$

Assume also that $\alpha = \beta$. This assumption is made for the sake of simplicity and also because, as is shown in Appendix IV, it corresponds to an anisotropic case in elasticity theory. Both u and v at the lattice point $i = 18$, $j = 1$ will be chosen equal to zero, and because of the symmetry of this specific case the conditions

$$\begin{aligned} u_{18,j} &= 0 \\ u_{18+k,j} &= -u_{18-k,j} \qquad k = 1,2, \ldots ,17 \qquad (2.50) \\ v_{18+k,j} &= v_{18-k,j} \end{aligned}$$

will be satisfied.

Due to this symmetry the number of unknowns and independent equations is halved and for this example equals 1139. The set of equations for this particular case is shown in Appendix IA. With such a large number of equations the only practical method of solution is an iteration procedure. The Seidel iteration technique [11] was applied to this system of equations using the Michigan State University Control Data 3600 digital computer. The iteration converged to a sufficiently accurate answer after approximately 13,000 iterations. At this point the greatest change for any of the 1139 unknowns for the last iteration was less than 10^{-9}.

An examination of this solution revealed that the assumption that the next nearest neighbor bonds between lattice points on the extra atom plane $i = r+1 = 18$ and the plane $i = r = 17$ have negligible rotation was unrealistic and should be corrected. This rotation is sufficiently taken account of by assuming that the bond between the lattice points $(r+1,s)$ and $(r,s-1)$, which for the particular numerical problem considered here correspond to (18,16) and (17,17) respectively, has a corrected slope of $r_y/r_x = 1/.8$. All other next nearest neighbor bonds between $i = r = 17$ and $i = r+1 = 18$ are assumed to have a corrected slope $r_y/r_x = 1/1$. The one exception is the bond between $(r+1,s)$ and $(r,s+1)$, i.e., (18,17) and (17,18) which retains its originally assumed slope of $r_y/r_x = 2/1$. The equilibrium equations which are altered by this change are shown in Appendix IB. The new system of equations was then programed for a Seidel iteration on the Control Data 3600 computer and after 13,000 iterations the greatest change in a variable for the last iteration was 2.5×10^{-10}. The displacement values for this solution are shown in Tables 1 and 2 and the Fortran program from which they were found is shown in Appendix VIII. The variations of u and v within various rows and columns of lattice points are graphically illustrated in Figures 15 through 18. The values of displacement shown in these figures are for the right half-lattice whereas the system in Appendix I whose solution appears in Tables 1 and 2 are for the left half-lattice. The only difference in the left and right half displacement values is a sign reversal for u. The index i = 18 in these figures corresponds to the extra atom plane while i = 1 still corresponds to the side boundary.

2.5. Calculation of Interplanar Forces

Besides checking the similarity of the continuum and discrete models by comparing their respective displacement fields another interesting comparison may be made between the stresses of the continuum model and analogous quantities for the discrete model.

These analogous quantities may be defined by passing a plane through the discrete model which separates it into two parts. The bond forces which act on lattice points on one side of this plane due only to interaction with those lattice points on the other side of the plane are the discrete counterparts of the continuum concept of stress. The bond force component which is normal to the plane corresponds to normal stress while the in-plane component corresponds to shear stress. For purposes of this dissertation the only plane considered will be

TABLE 1

u DISPLACEMENT FOR THE DISCRETE MODEL (b, FOR LEFT HALF CRYSTAL)

33	.12369	.12364	.12334	.12257	.12111	.11872	.11522	.11042	.10420	.09649	.08728	.07664	.06467	.05156	.03752	.02279	.00765	-
32	.09831	.09832	.09814	.09762	.09657	.09485	.09227	.08868	.08396	.07802	.07083	.06240	.05283	.04223	.03079	.01873	.00629	-
31	.07301	.07323	.07331	.07317	.07271	.07179	.07027	.06801	.06487	.06073	.05554	.04926	.04195	.03370	.02466	.01504	.00506	-
30	.04791	.04832	.04872	.04905	.04925	.04923	.04886	.04802	.04653	.04426	.04108	.03694	.03182	.02581	.01903	.01166	.00393	-
29	.02288	.02354	.02427	.02509	.02597	.02686	.02769	.02831	.02854	.02820	.02711	.02514	.02223	.01840	.01378	.00853	.00289	-
28	-.00207	-.00118	-.00014	.00112	.00264	.00441	.00639	.00846	.01045	.01212	.01322	.01352	.01288	.01127	.00877	.00556	.00191	-
27	-.02695	-.02587	-.02458	-.02295	-.02090	-.01837	-.01536	-.01192	-.00821	-.00449	-.00109	.00165	.00344	.00417	.00386	.00269	.00096	-
26	-.05176	-.05055	-.04908	-.04720	-.04477	-.04168	-.03784	-.03323	-.02794	-.02221	-.01641	-.01103	-.00653	-.00322	-.00117	-.00021	.00002	-
25	-.07648	-.07520	-.07365	-.07164	-.06901	-.06559	-.06121	-.05575	-.04919	-.04164	-.03346	-.02523	-.01766	-.01134	-.00658	-.00327	-.00097	-
24	-.10107	-.09981	-.09826	-.09625	-.09361	-.09011	-.08553	-.07966	-.07230	-.06338	-.05308	-.04192	-.03084	-.02089	-.01280	-.00670	-.00205	-
23	-.12552	-.12433	-.12287	-.12099	-.11850	-.11518	-.11076	-.10494	-.09740	-.08783	-.07606	-.06230	-.04743	-.03299	-.02055	-.01083	-.00333	-
22	-.14981	-.14874	-.14745	-.14580	-.14361	-.14068	-.13673	-.13143	-.12437	-.11504	-.10294	-.08764	-.06934	-.04960	-.03118	-.01629	-.00495	-
21	-.17395	-.17305	-.17197	-.17062	-.16886	-.16648	-.16325	-.15885	-.15285	-.14469	-.13360	-.11863	-.09881	-.07404	-.04753	-.02449	-.00726	-
20	-.19797	-.19726	-.19645	-.19547	-.19419	-.19248	-.19014	-.18690	-.18240	-.17612	-.16729	-.15477	-.13678	-.11095	-.07572	-.03924	-.01108	-
19	-.22193	-.22144	-.22092	-.22032	-.21959	-.21861	-.21725	-.21534	-.21260	-.20866	-.20293	-.19447	-.18163	-.16136	-.12775	-.07200	-.02054	-
18	-.24591	-.24564	-.24542	-.24524	-.24506	-.24485	-.24453	-.24401	-.24316	-.24179	-.23958	-.23604	-.23029	-.22053	-.20256	-.16336	-.05710	-
17	-.27001	-.26996	-.27005	-.27028	-.27066	-.27121	-.27194	-.27284	-.27393	-.27520	-.27667	-.27837	-.28037	-.28294	-.28687	-.29649	-.32615	0
16	-.29434	-.29451	-.29489	-.29551	-.29644	-.29774	-.29950	-.30181	-.30482	-.30874	-.31389	-.32082	-.33057	-.34528	-.36994	-.41553	-.50348	0
15	-.31900	-.31938	-.32003	-.32103	-.32248	-.32449	-.32723	-.33089	-.33575	-.34220	-.35086	-.36267	-.37931	-.40369	-.44023	-.49251	-.54279	0
14	-.34410	-.34466	-.34557	-.34691	-.34883	-.35148	-.35511	-.36000	-.36653	-.37525	-.38691	-.40261	-.42393	-.45259	-.48892	-.52676	-.55892	0
13	-.36972	-.37045	-.37156	-.37320	-.37551	-.37871	-.38309	-.38899	-.39687	-.40731	-.42103	-.43889	-.46158	-.48886	-.51803	-.54495	-.56735	0
12	-.39591	-.39677	-.39806	-.39991	-.40252	-.40614	-.41105	-.41764	-.42635	-.43770	-.45219	-.47012	-.49121	-.51406	-.53633	-.55597	-.57251	0
11	-.42269	-.42365	-.42505	-.42705	-.42984	-.43367	-.43883	-.44568	-.45458	-.46587	-.47973	-.49598	-.51383	-.53189	-.54871	-.56339	-.57596	0
10	-.45006	-.45107	-.45251	-.45455	-.45737	-.46120	-.46629	-.47289	-.48127	-.49155	-.50367	-.51719	-.53133	-.54510	-.55770	-.56875	-.57840	0
9	-.47797	-.47898	-.48039	-.48237	-.48506	-.48865	-.49330	-.49919	-.50641	-.51494	-.52458	-.53493	-.54540	-.55545	-.56464	-.57283	-.58013	0
8	-.50635	-.50730	-.50862	-.51042	-.51282	-.51594	-.51986	-.52463	-.53022	-.53653	-.54334	-.55037	-.55736	-.56406	-.57031	-.57605	-.58134	0
7	-.53513	-.53597	-.53711	-.53866	-.54061	-.54307	-.54603	-.54943	-.55315	-.55703	-.56089	-.56462	-.56820	-.57170	-.57519	-.57867	-.58212	0
6	-.56422	-.56491	-.56582	-.56698	-.56841	-.57009	-.57195	-.57386	-.57566	-.57714	-.57815	-.57865	-.57883	-.57905	-.57968	-.58086	-.58253	0
5	-.59397	-.59408	-.59471	-.59596	-.59628	-.59711	-.59783	-.59827	-.59823	-.59751	-.59591	-.59340	-.59018	-.58684	-.58419	-.58279	-.58259	0
4	-.62312	-.62344	-.62379	-.62410	-.62431	-.62429	-.62390	-.62297	-.62128	-.61861	-.61478	-.60965	-.60328	-.59611	-.58940	-.58469	-.58240	0
3	-.65285	-.65300	-.65307	-.65298	-.65261	-.65182	-.65043	-.64825	-.64511	-.64078	-.63509	-.62787	-.61896	-.60840	-.59680	-.58704	-.58215	0
2	-.68272	-.68274	-.68261	-.68220	-.68136	-.67990	-.67764	-.67440	-.66999	-.66424	-.65700	-.64813	-.63745	-.62470	-.60949	-.59205	-.58066	0
1	-.71271	-.71267	-.71245	-.71187	-.71072	-.70877	-.70582	-.70167	-.69615	-.68914	-.68054	-.67031	-.65638	-.64460	-.62849	-.60816	-.57767	0
j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18

TABLE 2

v DISPLACEMENT FOR THE DISCRETE MODEL (r, FOR LEFT HALF CRYSTAL)

j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
33	.47202	.44652	.42091	.39526	.36971	.34448	.31986	.29616	.27372	.25288	.23396	.21724	.20297	.19134	.18250	.17655	.17356	-
32	.47208	.44653	.42077	.39486	.36896	.34328	.31811	.29379	.27067	.24917	.22949	.21211	.19724	.18511	.17587	.16965	.16652	-
31	.47235	.44680	.42095	.39487	.36871	.34268	.31707	.29222	.26849	.24629	.22600	.20798	.19253	.17989	.17026	.16377	.16051	-
30	.47297	.44747	.42160	.39544	.36913	.34286	.31690	.29158	.26729	.24444	.22346	.20476	.18867	.17548	.16542	.15863	.15521	-
29	.47401	.44859	.42279	.39666	.37032	.34393	.31772	.29201	.26717	.24364	.22190	.20240	.18556	.17171	.16112	.15397	.15037	-
28	.47547	.45018	.42452	.39854	.37231	.34594	.31962	.29361	.26826	.24407	.22141	.20095	.18317	.16848	.15721	.14959	.14575	-
27	.47732	.45219	.42676	.40104	.37506	.34889	.32263	.29647	.27071	.24575	.22215	.20054	.18155	.16574	.15356	.14529	.14112	-
26	.47946	.45452	.42938	.40403	.37846	.35267	.32669	.30061	.27461	.24903	.22440	.20140	.18086	.16355	.15010	.14093	.13630	-
25	.48177	.45706	.43227	.40737	.38233	.35709	.33163	.30591	.27999	.25403	.22844	.20397	.18144	.16210	.14685	.13638	.13107	-
24	.48412	.45967	.43526	.41086	.38613	.36189	.33716	.31213	.28669	.26080	.23460	.20859	.18384	.16179	.14399	.13158	.12524	-
23	.48640	.46221	.43818	.41429	.39051	.36675	.34297	.31886	.29434	.26911	.24297	.21599	.18890	.16342	.14192	.12652	.11857	-
22	.48851	.46456	.44088	.41747	.39431	.37134	.34847	.32554	.30229	.27834	.25321	.22638	.19770	.16839	.14163	.12145	.11076	-
21	.49036	.46661	.44321	.42021	.39759	.37534	.35339	.33161	.30979	.28754	.26417	.23909	.21086	.17881	.14534	.11770	.10141	-
20	.49189	.46828	.44508	.42237	.40016	.37848	.35730	.33654	.31606	.29558	.27458	.25222	.22696	.19640	.15751	.11658	.09003	-
19	.49307	.46950	.44639	.42383	.40187	.38056	.35991	.33990	.32047	.30145	.28253	.26313	.24213	.21718	.18350	.12902	.07685	-
18	.49386	.47023	.44709	.42452	.40262	.38144	.36103	.34141	.32257	.30443	.28685	.26954	.25192	.23285	.20920	.17422	.07468	-
17	.49428	.47047	.44715	.42442	.40236	.38105	.36055	.33376	.32209	.30411	.28683	.27006	.25343	.23614	.21673	.18791	.13634	.04941
16	.49431	.47031	.44657	.42350	.40108	.37937	.35844	.32739	.31898	.30035	.28274	.26431	.24583	.22530	.19877	.15808	.07706	.04910
15	.49399	.46947	.44538	.42181	.39881	.37646	.35478	.31957	.31337	.29330	.27335	.25779	.23037	.20357	.16807	.11766	.06902	.05892
14	.49332	.46829	.44363	.41941	.39567	.37243	.34969	.31078	.30540	.28342	.26094	.23705	.21028	.17856	.14030	.10058	.07139	.06507
13	.49235	.46673	.44140	.41641	.39176	.36744	.34341	.30160	.29572	.27150	.24635	.21944	.18982	.15710	.12338	.09388	.07432	.07008
12	.49111	.46484	.43879	.41294	.38727	.36175	.33620	.29267	.28498	.25859	.23119	.20229	.17219	.14167	.11347	.09091	.07671	.07361
11	.48966	.46273	.43591	.40916	.38244	.35567	.32877	.28459	.27401	.24583	.21697	.18759	.15842	.13095	.10723	.08921	.07824	.07585
10	.48806	.46048	.43291	.40528	.37751	.34955	.32130	.27779	.26363	.23421	.20468	.17560	.14802	.12328	.10280	.08774	.07885	.07697
9	.48639	.45821	.42993	.40147	.37277	.34375	.31436	.27254	.25452	.22440	.19473	.16631	.14018	.11747	.09918	.08605	.07853	.07691
8	.48475	.45603	.42713	.39795	.36845	.33858	.30834	.26892	.24713	.21672	.18719	.15938	.13427	.11284	.09587	.08391	.07726	.07585
7	.48322	.45406	.42463	.39487	.36476	.33428	.30350	.27254	.24166	.21127	.18197	.15456	.12994	.10904	.09262	.08119	.07502	.07373
6	.48189	.45238	.42255	.39237	.36184	.33101	.29997	.26892	.22817	.20797	.17896	.15174	.12717	.10603	.08939	.07784	.07171	.07042
5	.48084	.45107	.42096	.39051	.35976	.32880	.29776	.26685	.23636	.20662	.17801	.15096	.12604	.10411	.08636	.07385	.06717	.06577
4	.48009	.45015	.41988	.38932	.35852	.32760	.29675	.26617	.23615	.20696	.17889	.15217	.12705	.10396	.08408	.06934	.06111	.05919
3	.47966	.44960	.41929	.38874	.35804	.32732	.29678	.26665	.23719	.20866	.18126	.15513	.13025	.10651	.08397	.06480	.05300	.05017
2	.47947	.44938	.41911	.38869	.35820	.32779	.29766	.26805	.23922	.21140	.18477	.15941	.13522	.11179	.08828	.06314	.04180	.03656
1	.47943	.44936	.41921	.38898	.35879	.32879	.29916	.27016	.24201	.21494	.18911	.16459	.14127	.11876	.09603	.07130	.03607	0

vertically oriented so that the discrete quantities will be analogous to σ_x and τ_{xy}.

Referring to Figure 9 consider the determination of the forces acting on the lattice points lying on the vertical plane i = k due to the interactions between these lattice points and lattice points lying to the left of i = k. For the simple model used in this problem the lattice point (k,j) experiences a resultant force due to the relative displacements of (k,j) and its three neighbors (k-1,j+1), (k-1,j), and (k-1,j-1). The component of this resultant force which is normal to the vertical plane is analogous to σ_x and will be called $F_x(j)$. The tangential component is analogous to τ_{xy} and will be called $F_{xy}(j)$. These lattice forces are shown in Figure 9 and referring to this figure the forces on the lattice points on i = k are

$$
\begin{aligned}
F_x(1) &= \alpha(u_{k,1} - u_{k-1,1}) + \frac{\beta}{2}(u_{k,1} - u_{k-1,2} - v_{k,1} + v_{k-1,2}) \\
F_{xy}(1) &= \frac{\beta}{2}(u_{k,1} - u_{k-1,2} - v_{k,1} + v_{k-1,2}) \\
F_x(j) &= \alpha(u_{k,j} - u_{k-1,j}) + \frac{\beta}{2}(u_{k,j} - u_{k-1,j+1} - v_{k,j} + \\
&\qquad v_{k-1,j+1}) + \frac{\beta}{2}(u_{k,j} - u_{k-1,j-1} + v_{k,j} - v_{k-1,j-1}) \qquad (2.51) \\
F_{xy}(j) &= \frac{\beta}{2}(u_{k,j} - u_{k-1,j+1} - v_{k,j} + v_{k-1,j+1}) - \frac{\beta}{2}(u_{k,j} - \\
&\qquad u_{k-1,j-1} + v_{k,j} - v_{k-1,j-1}) \\
F_x(n) &= \alpha(u_{k,n} - u_{k-1,n}) + \frac{\beta}{2}(u_{k,n} - u_{k-1,n-1} + v_{k,n} - \\
&\qquad v_{k-1,n-1})
\end{aligned}
$$

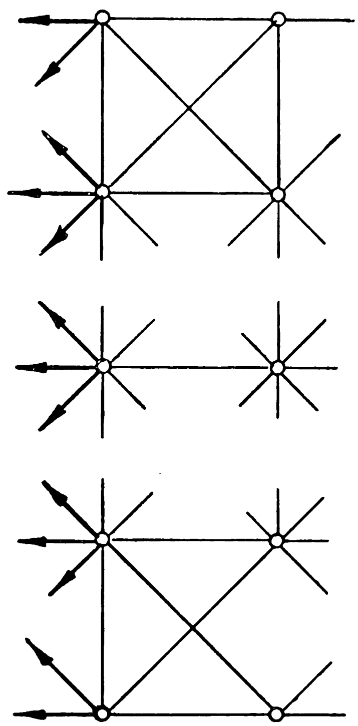


Fig. 9.--Lattice forces acting on the right hand portion of the lattice due to interaction with the left hand portion

$$F_{xy}(n) = -\frac{\beta}{2}(u_{k,n} - u_{k-1,n-1} + v_{k,n} - v_{k-1,n-1}).$$

The magnitudes of these forces for the example mentioned in Section 2.4 are shown in Table 3 for k = 5, 9, and 13. They are graphically represented in Figures 19 and 20.

It should be noted that the equations (2.51) are linearized force equations in which the squares of relative displacements have been neglected. Since these forces are calculated from a known displacement field it is not necessary

TABLE 3

LATTICE FORCES ACTING ACROSS A VERTICAL SECTION (αb)

j	i = 5		i = 9		i = 13	
	F_x	F_{xy}	F_x	F_{xy}	F_x	F_{xy}
33	-.00229	.00083	-.00849	.00227	-.01540	.00344
32	-.00215	.00141	-.00800	.00232	-.01507	.00168
31	-.00138	.00216	-.00552	.00386	-.01136	.00317
30	-.00058	.00259	-.00301	.00497	-.00770	.00447
29	.00021	.00270	-.00048	.00565	-.00401	.00559
28	.00090	.00252	.00201	.00587	-.00022	.00656
27	.00143	.00207	.00438	.00556	.00377	.00735
26	.00178	.00140	.00646	.00467	.00808	.00793
25	.00193	.00059	.00805	.00316	.01280	.00811
24	.00189	-.00027	.00893	.00109	.01797	.00758
23	.00171	-.00111	.00899	-.00138	.02333	.00573
22	.00142	-.00187	.00821	-.00401	.02788	.00168
21	.00109	-.00251	.00681	-.00648	.02930	-.00513
20	.00075	-.00299	.00505	-.00855	.02573	-.01377
19	.00042	-.00331	.00316	-.01005	.01795	-.02189
18	.00012	-.00347	.00128	-.01092	.00842	-.02727
17	-.00016	-.00348	-.00056	-.01113	-.00133	-.02890
16	-.00042	-.00334	-.00240	-.01068	-.01117	-.02655
15	-.00067	-.00306	-.00424	-.00956	-.02062	-.02058
14	-.00092	-.00264	-.00604	-.00779	-.02778	-.01227
13	-.00117	-.00208	-.00762	-.00545	-.03058	-.00385
12	-.00139	-.00141	-.00875	-.00273	-.02894	.00278
11	-.00156	-.00065	-.00915	.00009	-.02462	.00705
10	-.00165	.00014	-.00870	.00271	-.01937	.00946
9	-.00161	.00091	-.00742	.00484	-.01399	.01072
8	-.00142	.00159	-.00549	.00632	-.00870	.01132
7	-.00108	.00212	-.00319	.00708	-.00345	.01149
6	-.00061	.00244	-.00076	.00715	.00180	.01125
5	-.00004	.00252	.00159	.00662	.00698	.01042
4	.00060	.00235	.00378	.00561	.01164	.00877
3	.00122	.00191	.00579	.00421	.01521	.00631
2	.00179	.00123	.00763	.00248	.01758	.00342
1	.00185	.00069	.00766	.00215	.01588	.00395

to neglect these quantities. However, the differences in the forces calculated with and without the linearization are small. Also, since the displacement field was calculated assuming force linearization, it is certainly not logical to calculate interatomic forces using the nonlinearized force.

III. CONTINUUM MODEL OF AN EDGE DISLOCATION IN A RECTANGULAR CRYSTAL WITH CUBIC SYMMETRY

3.1. Problem Formulation

For the sake of comparison with the displacements found for the discrete dislocation model of the previous chapter, a similar calculation will be made using the traditional elastic continuum model. Since the discrete model considered in this dissertation does not correspond to an isotropic continuum (see Appendix IV), it will be necessary to use the anisotropic theory of elasticity with the elastic constants c_{11}, c_{12}, and c_{44}.

An edge dislocation is to be produced in the rectangular elastic continuum of Figure 10. This is accomplished by making a vertical cut of height h at a distance e from the lower left hand corner. After deleting a small cylinder of material at the root of the cut in order to remove the singularity which otherwise exists there, the two sides of the cut are displaced relative to one another by one atomic spacing in the x direction. A plane strain solution for the x and y displacements of the continuum is required. The form of the displacement functions for the general case of strain and for general anisotropy has been considered by Eshelby [5] and then

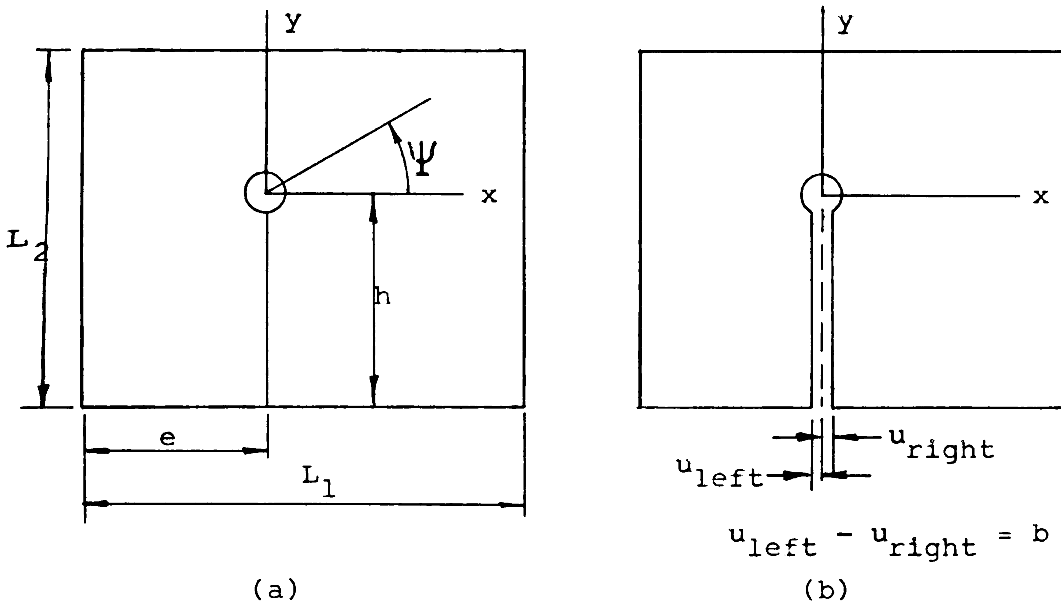


Fig. 10.--Formation of an elastic dislocation

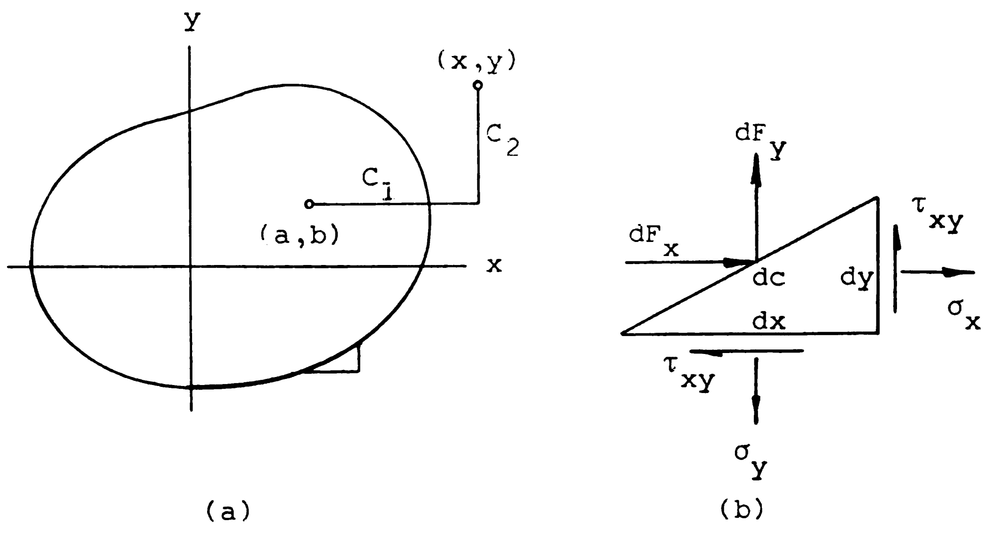


Fig. 11. Element lying on the closed boundary, C, of an elastic continuum

specialized for application to problems involving dislocations. It is shown in Appendix II that for the specific case of plane strain and cubic anisotropy the displacements have the form

$$
\begin{aligned}
u &= f_{(1)}[z_{(1)}] + f_{(2)}[z_{(2)}] \\
v &= A_{(1)} f_{(1)}[z_{(1)}] + A_{(2)} f_{(2)}[z_{(2)}]
\end{aligned}
\qquad (3.1)
$$

where

$$
\begin{aligned}
z_{(1)} &= x + e^{i\eta} y \\
z_{(2)} &= x - e^{i\eta} y
\end{aligned}
\qquad (3.2)
$$

$$
\begin{aligned}
A_{(1)} &= -A_{(2)} = -\frac{c_{11}e^{-i\eta} + c_{44}e^{i\eta}}{c_{12} + c_{44}} \\
\eta &= \tfrac{1}{2}\cos^{-1}\frac{(2c_{12}c_{44} + c_{12}^{2} - c_{11}^{2})}{2c_{11}c_{44}} .
\end{aligned}
\qquad (3.3)
$$

The functions $f_{(1)}$ and $f_{(2)}$ are determined by the boundary conditions of the particular problem. It is shown in Appendix II that the displacement discontinuity

$$u_{right} - u_{left} = b$$

along the negative x axis in Figure 10 may be satisfied if the functions have the form

$$
\begin{aligned}
f_{(1)}[z_{(1)}] &= \frac{D_{(1)}}{2\pi i}\log z_{(1)} \\
f_{(2)}[z_{(2)}] &= \frac{D_{(2)}}{2\pi i}\log z_{(2)}
\end{aligned}
\qquad (3.4)
$$

since the logarithmic function changes by the amount $2\pi i$ with every circuit of the origin. This form for $f_{(1)}$ and

$f_{(2)}$ does not, however, satisfy the stress-free condition on the rectangular boundaries of the elastic crystal. Indeed, this condition cannot be satisfied by any simple analytic function. In view of this fact, the solution will be made in two parts. The first part will consist of an analytic solution using the equations (3.4) as the form of $f_{(1)}$ and $f_{(2)}$. The second part consists of a numerical solution with boundary stresses which are equal but opposite to those resulting from the analytic solution. The superposition of these two solutions will result in the satisfaction of both boundary conditions.

3.2. Analytic Solution

It is shown in Appendix II that the displacements which satisfy the displacement discontinuity on the negative y axis have the form

$$
\begin{aligned}
u &= \mathrm{Re}\left[\frac{D_{(1)}}{2\pi i}\log z_{(1)} + \frac{D_{(2)}}{2\pi i}\log z_{(2)}\right] \\
v &= \mathrm{Re}\left[A_{(1)}\frac{D_{(1)}}{2\pi i}\log z_{(1)} + A_{(2)}\frac{D_{(2)}}{2\pi i}\log z_{(2)}\right]
\end{aligned}
\qquad (3.5)
$$

where the constants $D_{(1)}$ and $D_{(2)}$, which are in general complex, are determined by boundary conditions. In the succeeding portion of Section 3.2 any equality containing u, v, or their derivatives or integrals will be understood to equate only the real parts of the quantities involved even though the symbol $\mathrm{Re}\left[\quad\right]$ will, in general, be left out.

a) Displacement Boundary Conditions for the Determination of $D_{(1)}$ and $D_{(2)}$

On the negative y axis the displacements (3.5) must satisfy the conditions

$$u(-\tfrac{\pi}{2}) - u(\tfrac{3\pi}{2}) = b \tag{3.6}$$

$$v(-\tfrac{\pi}{2}) - v(\tfrac{3\pi}{2}) = 0. \tag{3.7}$$

It may be seen from the mapping of the xy plane onto the $w_{(2)} = \log z_{(2)}$ plane in Figure 31 of Appendix III that a positive (counter-clockwise) angle change of 2π in the xy plane causes a change in the value of $w_{(2)}$ of amount $-2\pi i$. Similarly, a positive change of angle 2π in the xy plane causes $w_{(1)} = \log z_{(1)}$ to change by amount $+2\pi i$ as may be seen from the mapping in Figure 32. With this in mind, a substitution of equations (3.5) into the boundary conditions (3.6) and (3.7) leads to the equations

$$D_{(2)} - D_{(1)} = b \tag{3.8}$$

$$A_{(2)}D_{(2)} - A_{(1)}D_{(1)} = 0. \tag{3.9}$$

The imaginary parts of these two equations have no significance for reasons already discussed. Therefore, only the two real equations associated with equations (3.8) and (3.9) are available for the solution of the two complex constants $D_{(1)}$ and $D_{(2)}$ where

$$\begin{aligned} D_{(1)} &= R_{(1)} + iI_{(1)} \\ D_{(2)} &= R_{(2)} + iI_{(2)}. \end{aligned} \tag{3.10}$$

Hence, two additional equations are necessary to determine $R_{(1)}$, $I_{(1)}$, $R_{(2)}$, and $I_{(2)}$.

b) Stress Boundary Conditions

Consider the equilibrium of that portion of a large body in static equilibrium which is included inside the contour C in the Figure 11a. If the element shown in Figure 11b is isolated from the larger body, equilibrium requires that the forces dF_x and dF_y which are transmitted across the elemental length dc must satisfy the equations

$$\begin{aligned} dF_x &= -\sigma_x dy + \tau_{xy} dx \\ dF_y &= \sigma_y dx - \tau_{xy} dy. \end{aligned} \tag{3.11}$$

If these expressions are integrated around the contour C, the result is the net x and y components of force transmitted by the material inside C to the material outside C. However, if the entire region is in equilibrium, then the material inside C is also in equilibrium so that the net force on C is zero.

$$\begin{aligned} \oint dF_x &= \oint -\sigma_x dy + \tau_{xy} dx = 0 \\ \oint dF_y &= \oint \sigma_y dx - \tau_{xy} dy = 0. \end{aligned} \tag{3.12}$$

The vanishing of these integrals regardless of the path C (as long as it is closed) implies the existence of two potential functions ϕ_x and ϕ_y such that

$$\oint d\phi_x = \oint \frac{\partial \phi_x}{\partial x} dx + \frac{\partial \phi_x}{\partial y} dy = \oint -\sigma_x dy + \tau_{xy} dx \tag{3.13a}$$

$$\oint d\phi_y = \oint \frac{\partial \phi_y}{\partial x}\, dx + \frac{\partial \phi_y}{\partial y}\, dy = \oint \sigma_y dx - \tau_{xy} dy. \tag{3.13b}$$

Equating coefficients of dx and dy in equations (3.13) gives

$$\sigma_x = -\frac{\partial \phi_x}{\partial y} \qquad \text{(a)}$$

$$\tau_{xy} = \frac{\partial \phi_x}{\partial x} = -\frac{\partial \phi_y}{\partial y} \qquad \text{(b)} \tag{3.14}$$

$$\sigma_y = \frac{\partial \phi_y}{\partial x}. \qquad \text{(c)}$$

The functions ϕ_x and ϕ_y may be found by integration of the perfect differentials of ϕ_x and ϕ_y along the path C_1C_2 in Figure 11a. To find ϕ_x integrate the expression

$$d\phi_x = \frac{\partial \phi_x}{\partial x}\, dx + \frac{\partial \phi_x}{\partial y}\, dy$$

along C_1C_2

$$\phi_x = \underbrace{\int_a^x \frac{\partial \phi_x}{\partial x}\, dx}_{y\,=\,b} + \underbrace{\int_b^y \frac{\partial \phi_x}{\partial y}\, dy}_{x\,=\,x}. \tag{3.15}$$

The first integral in (3.15) is a function of x only since y = b along path C_1, while the second is a function of both x and y which may be found by an indefinite integration of $\frac{\partial \phi_x}{\partial y}$ with respect to y. The function ϕ_x then may be written

$$\phi_x = \Theta(x) + F(x,y) \tag{3.16}$$

where

$$F(x,y) = \int \frac{\partial \phi_x}{\partial y}\, dy. \tag{3.17}$$

Differentiating equation (3.16) with respect to x gives

$$\frac{\partial \phi_x}{\partial x} = \Theta'(x) + \frac{\partial F}{\partial x}$$

or

$$\Theta'(x) = \frac{\partial \phi_x}{\partial x} - \frac{\partial F}{\partial x}. \tag{3.18}$$

Equation (3.18) may now be integrated indefinitely with respect to x to find $\Theta(x)$

$$\Theta(x) = \int \left(\frac{\partial \phi_x}{\partial x} - \frac{\partial F}{\partial x}\right) dx. \tag{3.19}$$

This procedure is outlined in Advanced Calculus by Taylor [12]. For the present situation

$$\frac{\partial \phi_x}{\partial x} = \tau_{xy} = c_{44}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)$$

$$\frac{\partial \phi_x}{\partial y} = -\sigma_x = -\left(c_{11}\frac{\partial u}{\partial x} + c_{12}\frac{\partial v}{\partial y}\right) \tag{3.20}$$

where u and v are given by equations (3.5). Substituting the appropriate derivatives into equations (3.20) gives

$$\frac{\partial \phi_x}{\partial x} = c_{44}\left[\frac{D_{(1)}}{2\pi i}\;\frac{e^{i\eta} + A_{(1)}}{x + e^{i\eta}y} - \frac{D_{(2)}}{2\pi i}\;\frac{e^{i\eta} - A_{(2)}}{x - e^{i\eta}y}\right] \tag{3.21}$$

$$\frac{\partial \phi_x}{\partial y} = -\left[\frac{D_{(1)}}{2\pi i}\;\frac{c_{11} + c_{12}A_{(1)}e^{i\eta}}{x + e^{i\eta}y} + \frac{D_{(2)}}{2\pi i}\;\frac{c_{11} - c_{12}A_{(2)}e^{i\eta}}{x - e^{i\eta}y}\right]. \tag{3.22}$$

Substituting expression (3.22) into equation (3.17) gives

$$F(x,y) = -\frac{D_{(1)}}{2\pi i}(c_{11} + c_{12}A_{(1)}e^{i\eta})\int\frac{dy}{x + e^{i\eta}y} -$$

$$\frac{D_{(2)}}{2\pi i}(c_{11} - c_{12}A_{(2)}e^{i\eta})\int\frac{dy}{x - e^{i\eta}y} \tag{3.23}$$

$$F(x,y) = -\frac{D_{(1)}}{2\pi i}\frac{[c_{11} + c_{12}A_{(1)}e^{i\eta}]}{e^{i\eta}}\log(x + e^{i}y) +$$

$$\frac{D_{(2)}}{2\pi i}\frac{[c_{11} - c_{12}A_{(2)}e^{i\eta}]}{e^{i\eta}}\log(x - e^{i\eta}y). \tag{3.24}$$

Differentiating equation (3.24) with respect to x

$$\frac{\partial F(x,y)}{\partial x} = -\frac{D_{(1)}}{2\pi i}\frac{[c_{11} + c_{12}A_{(1)}e^{i\eta}]}{e^{i\eta}}\frac{1}{x + e^{i\eta}y} +$$

$$\frac{D_{(2)}}{2\pi i}\frac{[c_{11} - c_{12}A_{(2)}e^{i\eta}]}{e^{i\eta}}\frac{1}{x - e^{i\eta}y}. \tag{3.25}$$

Substituting the expressions (3.21) and (3.25) into equation (3.19)

$$\Theta(x) = \int\frac{D_{(1)}}{2\pi i}\frac{[c_{44}e^{i\eta} + c_{44}A_{(1)} + c_{11}e^{-i\eta} + c_{12}A_{(1)}]}{x + e^{i\eta}y} -$$

$$\frac{D_{(2)}}{2\pi i}\frac{[c_{44}e^{i\eta} - c_{44}A_{(2)} + c_{11}e^{-i\eta} - c_{12}A_{(2)}]}{x - e^{i\eta}y}dx \tag{3.26}$$

$$\Theta(x) = \frac{D_{(1)}}{2\pi i}[c_{44}e^{i\eta} + c_{44}A_{(1)} + c_{11}e^{-i\eta} + c_{12}A_{(1)}]$$

$$\log(x + e^{i\eta}y) - \frac{D_{(2)}}{2\pi i}[c_{44}e^{i\eta} - c_{44}A_{(2)} + c_{11}e^{-i\eta} -$$

$$c_{12}A_{(2)}]\log(x - e^{i\eta}y).$$

Now substituting $\Theta(x)$ and $F(x,y)$ into the equation (3.16) gives

$$\phi_x = \frac{D_{(1)}}{2\pi i} c_{44}[e^{i\eta} + A_{(1)}] \log (x + e^{i\eta}y) -$$

$$\frac{D_{(2)}}{2\pi i} c_{44}[e^{i\eta} - A_{(2)}] \log (x - e^{i\eta}y). \tag{3.27}$$

In a similar manner the potential function ϕ_y is found to be

$$\phi_y = \frac{D_{(1)}}{2\pi i} [c_{11}e^{i\eta}A_{(1)} + c_{12}] \log (x + e^{i\eta}y) +$$

$$\frac{D_{(2)}}{2\pi i} [-c_{11}e^{i\eta}A_{(2)} + c_{12}] \log (x - e^{i\eta}y). \tag{3.28}$$

Equilibrium requires that the integral of these functions ϕ_x and ϕ_y about any closed path be zero. If, for example, the path starts at $\Psi = -\frac{\pi}{2}$ and ends at the same point at $\Psi = \frac{3\pi}{2}$, the conditions for static equilibrium are

$$\begin{aligned} \oint d\phi_x &= \phi_x \left(\tfrac{3\pi}{2}\right) - \phi_x \left(-\tfrac{\pi}{2}\right) \\ \oint d\phi_y &= \phi_y \left(\tfrac{3\pi}{2}\right) - \phi_y \left(-\tfrac{\pi}{2}\right). \end{aligned} \tag{3.29}$$

Substituting equations (3.27) and (3.28) into the boundary conditions (3.29) and noting that $\log (x + e^{i\eta}y)$ changes value by the amount $+2\pi i$ and $\log (x - e^{i\eta}y)$ changes value by the amount $-2\pi i$ as Ψ changes by $+2\pi$, the following equations result:

$$D_{(1)}[e^{i\eta} + A_{(1)}] + D_{(2)}[e^{i\eta} - A_{(2)}] = 0 \tag{3.30}$$

$$D_{(1)}[c_{11}e^{i\eta}A_{(1)} + c_{12}] - D_{(2)}[-c_{11}e^{i\eta}A_{(2)} + c_{12}] = 0. \tag{3.31}$$

It is shown in Appendix II that

$$A_{(2)} = -A_{(1)}.$$

Making this substitution into equations (3.30) and (3.31) gives the equations

$$[D_{(1)} + D_{(2)}][e^{i\eta} + A_{(1)}] = 0 \tag{3.32}$$

$$[D_{(1)} - D_{(2)}][c_{11}A_{(1)}e^{i\eta} + c_{12}] = 0 \tag{3.33}$$

which, together with equations (3.8) and (3.9) may be solved for the real and imaginary parts of $D_{(1)}$ and $D_{(2)}$.

The simultaneous solution of the four boundary condition equations using only the real parts of these equations gives

$$D_{(1)} = -D_{(2)} = -.5b(1 - ik_1) \tag{3.34}$$

where the constant k_1 is given by

$$k_1 = \frac{c_{12}{}^2 + c_{12}c_{44} - c_{11}{}^2 - c_{11}c_{44}\cos 2\eta}{c_{11}c_{44}\sin 2\eta}. \tag{3.35}$$

The value of $D_{(1)}$ and $D_{(2)}$ given by equation (3.34) with k_1 given by equation (3.35) are different from those found by Eshelby [5]. The displacements for an edge dislocation in an unbounded continuum with cubic anisotropy are given by the real parts of the following equations:

$$u = \frac{b}{4\pi}(k_1 + i)[\log z_{(1)} - \log z_{(2)}] + H_1 \tag{3.36}$$

$$v = \frac{b}{4\pi}(k_1 + i)\, A_{(1)}\, [\log z_{(1)} + \log z_{(2)}] + H_2. \tag{3.37}$$

The constants H_1 and H_2 are determined by the rigid body position of the unbounded medium. For comparison with the displacements of the discrete model, the u displacement will be symmetrical about the y axis and the v displacement will be made zero at some point on the negative y axis. The boundary conditions for displacement are

$$u(-\frac{\pi}{2}) = -u(\frac{3\pi}{2}) = b/2 \tag{3.38}$$

$$v(0,L) = 0. \tag{3.39}$$

Referring to the transformation diagrams, Figures 31 and 32 in Appendix III, a point (0,y) on the negative y axis maps on the point $\log y + i(\eta + \pi)$ in the $\log z_{(1)}$ plane and on the point $\log y + i\eta$ in the $\log z_{(2)}$ plane so that the condition (3.39) leads to the equation

$$\frac{b}{2} = \frac{b}{4\pi}(k_1 + i)\,[\log y + i(\eta + \pi) - \log y - i\eta] + H_1.$$

Expanding this expression and ignoring the imaginary portion gives

$$H_1 = 3b/4. \tag{3.40}$$

The condition (3.39) leads to the equation

$$0 = \frac{b}{4\pi}(k_1 + i)A_{(1)}[\log L + i(\eta + \pi) + \log L + i\ ] + H_2 \tag{3.41}$$

where

$$A_{(1)} = -\frac{c_{11}e^{-i\eta} + c_{44}e^{i\eta}}{c_{12} + c_{44}} = -\frac{c_{11} + c_{44}}{c_{12} + c_{44}}\cos\eta + i$$

$$\frac{c_{11} - c_{44}}{c_{12} + c_{44}}\sin\eta$$

or making the substitutions

$$k_2 = \frac{c_{11} + c_{44}}{c_{12} + c_{44}} \cos\eta , \qquad k_3 = \frac{c_{11} - c_{44}}{c_{12} + c_{44}} \sin\eta$$

$$A_{(1)} = -k_2 + ik_3.$$

Substituting this value of $A_{(1)}$ into (3.41) gives

$$H_2 = -\frac{b}{4\pi}(k_1 + i)(-k_2 + ik_3)[2 \log L + i(2\eta + \pi)].$$

Expanding this expression and discarding the imaginary portion gives

$$H_2 = \frac{b}{4\pi}[(k_1k_2 + k_3) \log L^2 + (k_1k_3 - k_2)(2\eta + \pi)]. \tag{3.42}$$

Then for the case of symmetrical u displacement and a zero v displacement at the point (0,-L) the displacement field of the edge dislocation in an infinite continuum is given by the equations

$$u = \mathrm{Re}\left(\frac{b}{4\pi}(k_1 + i)[\log z_{(1)} - \log z_{(2)}] + 3b/4\right) \tag{3.43}$$

$$v = \mathrm{Re}\left(\frac{b}{4\pi}[(-k_1k_2 - k_3) + i(k_3k_1 - k_2)][\log z_{(1)} + \log z_{(2)}] + \frac{b}{4\pi}[(k_1k_2 + k_3) \log L^2 + (k_1k_3 - k_2)(2\eta + \pi)]\right). \tag{3.44}$$

If the logarithmic functions of the complex variables are expressed in complex form, that is

$$\log z_{(1)} = r_{(1)} + is_{(1)}$$

$$\log z_{(2)} = r_{(2)} + is_{(2)},$$

and if the equations (3.43) and (3.44) are expanded, u and v may be written in the form

$$u = \frac{b}{4\pi} \left(k_1[r_{(1)} - r_{(2)}] - [s_{(1)} - s_{(2)}] + 3\pi \right) \tag{3.45}$$

$$v = \frac{b}{4\pi} \left([-k_1k_2 - k_3][r_{(1)} + r_{(2)} - 2 \log L] - \right.$$

$$\left. [k_3k_1 - k_2][s_{(1)} + s_{(2)} - 2\eta - \pi] \right) . \tag{3.46}$$

The real portions of log $z_{(1)}$ and log $z_{(2)}$ are given by the equations

$$r_{(1)} = \frac{1}{2} \log (x^2 + y^2 + 2xy \cos\eta) \tag{3.47}$$

$$r_{(2)} = \frac{1}{2} \log (x^2 + y^2 - 2xy \cos\eta) \tag{3.48}$$

while the imaginary portions may be determined with the help of the transformation diagrams, Figures 31 and 32, in Appendix III. The stresses associated with the displacements given in equations (3.43) and (3.44) may be determined by the application of the definitions of stress in terms of displacement.

$$\sigma_x = c_{11} \frac{\partial u}{\partial x} + c_{12} \frac{\partial v}{\partial y} \tag{3.49}$$

$$\sigma_y = c_{12} \frac{\partial u}{\partial x} + c_{11} \frac{\partial v}{\partial y} \tag{3.50}$$

$$\tau_{xy} = c_{44}(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}) . \tag{3.51}$$

The resulting stresses are

$$\sigma_x = b \frac{y(C_1x^2 + C_2y^2)}{x^4 + Dx^2y^2 + y^4} \tag{3.52}$$

$$\sigma_y = b \frac{C_3y(y^2 - x^2)}{x^4 + Dx^2y^2 + y^4} \tag{3.53}$$

$$\tau_{xy} = b\,\frac{x(C_4x^2 + C_5y^2)}{x^4 + Dx^2y^2 + y^4} \tag{3.54}$$

where

$$C_1 = \frac{1}{2\pi}\Bigg\{-\Bigg[\left(\frac{c_{12}^{\ 2} + c_{12}c_{44} - c_{11}^{\ 2} - c_{11}c_{44}\cos 2\eta}{c_{11}c_{44}\sin 2\eta}\right)$$

$$\left(\frac{c_{11}c_{44} - c_{12}c_{44}\cos 2\eta}{c_{12} + c_{44}}\right) + \frac{c_{12}c_{44}}{c_{12} + c_{44}}\sin 2\eta\Bigg]\cos\eta\ -$$

$$\Bigg[\left(\frac{c_{12}^{\ 2} + c_{12}c_{44} - c_{11}^{\ 2} - c_{11}c_{44}\cos 2\eta}{c_{11}c_{44}\sin 2\eta}\right)\left(\frac{c_{12}c_{44}}{c_{12} + c_{44}}\right)$$

$$\sin 2\eta\ -\ \frac{c_{11}c_{44} - c_{12}c_{44}\cos 2\eta}{c_{12} + c_{44}}\Bigg]\sin\eta\Bigg\} \tag{3.55}$$

$$C_2 = \frac{1}{2\pi}\Bigg\{\Bigg[\left(\frac{c_{12}^{\ 2} + c_{12}c_{44} - c_{11}^{\ 2} - c_{12}c_{44}\cos 2\eta}{c_{11}c_{44}\sin 2\eta}\right)$$

$$\left(\frac{c_{11}c_{44} - c_{12}c_{44}\cos 2\eta}{c_{12} + c_{44}}\right) + \frac{c_{12}c_{44}}{c_{12} + c_{44}}\sin 2\eta\Bigg]\cos\eta\ -$$

$$\Bigg[\left(\frac{c_{12}^{\ 2} + c_{12}c_{44} - c_{11}^{\ 2} - c_{12}c_{44}\cos 2\eta}{c_{11}c_{44}\sin 2\eta}\right)\Bigg(\frac{c_{12}c_{44}}{c_{12} + c_{44}}$$

$$\sin 2\eta\Bigg) - \frac{c_{11}c_{44} - c_{12}c_{44}\cos 2\eta}{c_{12} + c_{44}}\Bigg]\sin\eta\Bigg\}$$

$$C_3 = \frac{1}{2\pi}\Bigg[\frac{(c_{12}^{\ 2} + c_{12}c_{44} - c_{11}^{\ 2} - c_{12}c_{44}\cos 2\eta)^2}{(c_{12} + c_{44})(c_{11}c_{44}\sin 2\eta)}\ +$$

$$\frac{c_{11}c_{44}}{c_{12} + c_{44}}\sin 2\eta\Bigg]\cos\eta$$

$$C_4 = \frac{c_{44}}{2\pi}\Bigg[-\frac{(c_{12}^{\ 2} + c_{12}c_{44} - c_{11}^{\ 2} - c_{12}c_{44}\cos 2\eta)}{(c_{11}c_{44}\sin 2\eta)}$$

$$\frac{(c_{11} - c_{12})}{(c_{12} + c_{44})}\cos\eta\ - \frac{c_{11} + c_{12}}{c_{12} + c_{44}}\sin\eta\Bigg] \tag{3.57}$$

$$C_5 = \frac{c_{44}}{2\pi}\left\{ - \left[\frac{(c_{12}^2 + c_{12}c_{44} - c_{11}^2 - c_{12}c_{44}\cos 2\eta)}{(c_{11}c_{44}\sin 2\eta)} \right.\right.$$

$$\left. \frac{(c_{11} - c_{12})}{(c_{12} + c_{44})}\cos\eta + \frac{c_{11} + c_{12}}{c_{12} + c_{44}}\sin\eta \right] [1 - 2\cos^2\eta] -$$

$$2\left[\frac{(c_{12}^2 + c_{12}c_{44} - c_{11}^2 - c_{12}c_{44}\cos 2\eta)}{(c_{11}c_{44}\sin 2\eta)} \right.$$

$$\left.\left. \frac{(c_{11} + c_{12})}{(c_{12} + c_{44})}\sin\eta - \frac{c_{11} - c_{12}}{c_{12} + c_{44}}\cos\eta \right] \sin\eta \cos\eta \right\} \qquad (3.58)$$

$$D = 2(1 - 2\cos^2\eta). \qquad (3.59)$$

The similarity between the equations for stress in the anisotropic case and the isotropic case may be seen by comparing equations (3.52) through (3.54) with the equations given on page 116 of Read [12]. The isotropic case requires the special condition $\cos\eta = 0$ or $\eta = \pm\frac{\pi}{2}$. In Appendix IV it is shown that the relationship between the constants α and β of the discrete model and the constants c_{11}, c_{12}, c_{44} of the continuum model are

$$c_{11} = b^2(\alpha + \beta)$$

$$c_{44} = b^2\beta$$

$$c_{12} + c_{44} = 2b^2\beta.$$

For the special case $\alpha = \beta$ which is used for the discrete model solution these conditions reduce to

$$c_{11} = 2b^2\alpha$$

$$c_{12} = c_{44} = b^2\alpha$$

or

$$c_{12} = c_{44} = \frac{c_{11}}{2} \text{ .} \qquad (3.60)$$

When the elastic moduli are related by the relationship (3.60), the various constants in the solution have the following values

$$\begin{aligned}
\cos 2\eta &= -.25 \\
\sin 2\eta &= .96824584 \\
\eta &= .91173829 \text{ rad} \\
\sin\eta &= .79056942 \\
\cos\eta &= .61237244 \\
C_1 &= .11324073\ c_{11} \qquad (3.61) \\
C_2 = C_3 = -C_4 = C_5 &= .07549382\ c_{11} \\
D &= .5 \\
k_1 &= \frac{-.750}{(.9375)^{1/2}} \\
-k_1k_2 - k_3 &= 0.316227 \\
k_3k_1 - k_2 &= -1.224744.
\end{aligned}$$

The displacements and stresses for this particular case are shown in Tables 4 through 8. Curves showing the variation of displacements and stresses are shown in Appendix IX.

3.3. Numerical Solution

Suppose that the crystal shown in Figure 10 is square and that the dislocation is symmetrically placed. The geometrical parameters of the problem may then be simplified to

TABLE 4

u DISPLACEMENTS FOR ANALYTIC SOLUTION (b)

1.	0	.00641	.01347	.02175	.03156	.04287	.05530	.06825	.08107
.875	0	.00736	.01569	.02576	.03786	.05167	.06639	.08107	.09495
.750	0	.00866	.01883	.03156	.04692	.06392	.08107	.09716	.11155
.625	0	.01053	.02359	.04050	.06046	.08107	.10018	.11680	.13082
.500	0	.01347	.03156	.05530	.08107	.10459	.12412	.13980	.15237
.375	0	.01883	.04692	.08107	.11155	.13496	.15237	.16549	.17563
.250	0	.03156	.08107	.12412	.15237	.17087	.18365	.19294	.19997
.125	0	.08107	.15237	.18365	.19997	.20988	.21653	.22129	.22487
0	–	.25000	.25000	.25000	.25000	.25000	.25000	.25000	.25000
– .125	.50000	.41893	.34763	.31635	.30003	.29012	.28347	.27871	.27513
– .250	.50000	.46844	.41893	.37588	.34763	.32913	.31635	.30706	.30003
– .375	.50000	.48117	.45308	.41893	.38845	.36504	.34763	.33451	.32437
– .500	.50000	.48653	.46844	.44470	.41893	.39541	.37588	.36020	.34763
– .625	.50000	.48947	.47641	.45950	.43954	.41893	.39982	.38320	.36918
– .750	.50000	.49134	.48117	.46844	.45308	.43608	.41893	.40284	.38845
– .875	.50000	.49264	.48306	.47424	.46214	.44833	.43361	.41893	.40505
–1.	.50000	.49360	.48653	.47825	.46844	.45713	.44697	.43175	.41893
y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.

TABLE 5

v DISPLACEMENTS FOR ANALYTIC SOLUTION (b, v IS SYMMETRIC WITH RESPECT TO y_1 = 0)

y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.
0	-	.02381	.05870	.07910	.09358	.10481	.11399	.12175	.12847
- .125	-.10465	-.02889	.03903	.06976	.08822	.10134	.11157	.11996	.12710
- .250	-.06977	-.04578	.00599	.04750	.07391	.09166	.10464	.11480	.12310
- .375	-.04936	-.03837	-.00894	.02640	.05606	.07804	.09432	.10682	.11681
- .5	-.03489	-.02865	-.01089	.01443	.04088	.06389	.08238	.09704	.10880
- .625	-.02365	-.01965	-.00798	.00990	.03106	.05211	.07088	.08673	.09988
- .750	-.01448	-.01169	-.00349	.00952	.02594	.04383	.06128	.07713	.09094
- .875	-.00672	-.00467	.00140	.01183	.02400	.03875	.05414	.06904	.08274
-1.	0	.00157	.00624	.01383	.02399	.03610	.04931	.06277	.07576

TABLE 6

σ_x FOR ANALYTIC SOLUTION ($\frac{bc_{11}}{L}$, σ_x IS ANTISYMMETRIC WITH RESPECT TO $y_1 = 0$)

y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.
0		0	0	0	0	0	0	0	0
- .125	-.60395	-.60395	-.22251	-.10124	-.05698	-.03642	-.02526	-.01854	-.01419
- .250	-.30198	-.34966	-.30198	-.18381	-.11125	-.07254	-.05062	-.03722	-.02843
- .375	-.20132	-.21994	-.23633	-.20132	-.14619	-.10293	-.07417	-.05531	-.04261
- .5	-.15099	-.15953	-.17483	-.17424	-.15099	-.11956	-.09191	-.07091	-.05563
- .625	-.12079	-.12533	-.13547	-.14204	-.13688	-.12079	-.10062	-.08175	-.06618
- .750	-.10066	-.10334	-.10997	-.11359	-.11816	-.11233	-.10065	-.08666	-.0730[illegible]
- .875	-.08628	-.08799	-.09245	-.09777	-.10122	-.10051	-.09510	-.08628	-.076[illegible]1
-1.	-.07549	-.07665	-.07977	-.08386	-.08741	-.08883	-.08712	-.08237	-.07549

TABLE 7

σ_y FOR ANALYTIC SOLUTION ($\frac{bc_{11}}{L}$, σ_y IS ANTISYMMETRICAL WITH RESPECT TO $y_1 = 0$)

y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.
0		0	0	0	0	0	0	0	0
− .125	−.60395	0	.09536	.05586	.03419	.02270	.01607	.01195	.00922
− .250	−.30198	−.19072	0	.05252	.04768	.03671	.02793	.02161	.01709
− .375	−.20132	−.16757	−.07878	0	.03101	.03542	.03179	.02682	.02232
− .500	−.15099	−.13674	−.09536	−.04135	0	.02011	.02626	.02615	.02384
− .625	−.12079	−.11351	−.09177	−.05903	−.02514	0	.01401	.01992	.02133
− .750	−.10066	−.09645	−.08379	−.06357	−.03939	−.01681	0	.01029	.01550
− .875	−.08628	−.08362	−.07564	−.06257	−.04576	−.02789	−.01200	0	.00786
−1.	−.07549	−.07372	−.06837	−.05952	−.04768	−.03413	−.02067	−.00899	0

TABLE 8

τ_{xy} FOR ANALYTIC SOLUTION $(\frac{bc_1}{L}$, τ_{xy} IS SYMMETRICAL WITH RESPECT TO $y_1 = 0)$

0	0	-.60395	-.30198	-.20132	-.15099	-.12079	-.10066	-.08628	-.07549
- .125	0	0	-.19072	-.16757	-.13674	-.11351	-.09645	-.08363	-.07372
- .250	0	.09536	0	-.07878	-.09536	-.09177	-.08379	-.07564	-.06837
- .375	0	.05586	.05252	0	-.04135	-.05903	-.06357	-.06257	-.05952
- .500	0	.03419	.04768	.03101	0	-.02514	-.03939	-.04576	-.04768
- .625	0	.02270	.03671	.03542	.02011	0	-.01681	-.02789	-.03413
- .750	0	.01607	.02793	.03179	.02626	.01401	0	-.01200	-.02067
- .875	0	.01195	.02161	.02682	.02615	.01992	.01029	0	-.00899
-1.	0	.00922	.01709	.02232	.02384	.02133	.01550	.00786	0
y_1 / x_1	0	.125	.250	.375	.500	.625	.750	.875	1.

$$L_1 = 2L$$

$$L_2 = 2L$$

$$e = L$$

$$h = L.$$

The stresses on the square boundary of the region $-L \leq x \leq L$, $-L \leq y \leq L$ corresponding to the analytic solution of Section 3.2 are evaluated from equations (3.52) through (3.54).

On the top boundary $y = L$

$$\left.\begin{aligned} \sigma_y &= bC_2L \frac{(L^2 - x^2)}{x^4 + DL^2x^2 + L^4} \\ \tau_{xy} &= bC_2 \frac{L^2x - x^3}{x^4 + DL^2x^2 + L^4} . \end{aligned}\right\} \quad (3.62)$$

On the side boundary $x = L$

$$\left.\begin{aligned} \sigma_x &= b \frac{C_1L^2y + C_2y^3}{y^4 + DL^2y^2 + L^4} \\ \tau_{xy} &= bLC_2 \frac{(y^2 - L^2)}{y^4 + DL^2y^2 + L^4}. \end{aligned}\right\} \quad (3.63)$$

On the bottom boundary $y = -L$

$$\left.\begin{aligned} \sigma_y &= bC_2L \frac{(x^2 - L^2)}{x^4 + DL^2x^2 + L^4} \\ \tau_{xy} &= bC_2 \frac{(L^2x - x^3)}{x^4 + DL^2x^2 + L^4}. \end{aligned}\right\} \quad (3.64)$$

On the side boundary $x = -L$

$$\left.\begin{aligned} \sigma_x &= b \frac{C_1L^2y + C_2y^3}{y^4 + DL^2y^2 + L^4} \\ \tau_{xy} &= b \frac{C_2L(L^2 - y^2)}{y^4 + DL^2y^2 + L^4}. \end{aligned}\right\} \quad (3.65)$$

Now, using a finite difference analysis, the solution for a square continuum of width and length 2L with boundary stresses which are equal but opposite to those of equations (3.62) through (3.65) will be found. Due to the symmetry of the boundary stress distribution the u displacement on the y axis may be assumed to be zero. Also, the v displacement at the point (0,-L) may be arbitrarily taken as zero. When this finite difference solution and the analytic solution of Section 3.2 are superimposed, both the displacement boundary conditions on the y axis and the zero stress solution on the boundary will be satisfied.

a) Problem Formulation

For the sake of convenience the dimensionless coordinates

$$x_1 = x/L$$

$$y_1 = y/L$$

are substituted into the stress equations (3.62) through (3.64). The appropriate stresses are evaluated on the planes $x_1 = \pm 1$ and $y_1 = \pm 1$ and these quantities, with signs reversed, are then used as the boundary tractions for the numerical solution. These boundary tractions are given by the following equations. On $y_1 = 1$

$$\sigma_y = \frac{b}{L} C_2 \frac{(x_1^2 - 1)}{x_1^4 + Dx_1^2 + 1} \tag{3.66}$$

$$\tau_{xy} = \frac{b}{L} C_2 \frac{(x_1^3 - x_1)}{x_1^4 + Dx_1^2 + 1}. \tag{3.67}$$

On $x_1 = 1$

$$\sigma_x = \frac{b}{L} \frac{-C_1 y_1 - C_2 y_1^3}{y_1^4 + D y_1^2 + 1} \tag{3.68}$$

$$\tau_{xy} = \frac{b}{L} C_2 \frac{1 - y_1^2}{y_1^4 + D y_1^2 + 1} \, . \tag{3.69}$$

On $y_1 = -1$

$$\sigma_y = \frac{b}{L} C_2 \frac{1 - x_1^2}{x_1^4 + D x_1^2 + 1} \tag{3.70}$$

$$\tau_{xy} = \frac{b}{L} C_2 \frac{x_1^3 - x_1}{x_1^4 + D x_1^2 + 1} . \tag{3.71}$$

The boundary stresses, which are shown in Figure 12, are symmetrical about the y_1 or y axis so that only the region for which x_1 or x is positive will be considered in the solution. The equation (3.14b)

$$\tau_{xy} = \frac{\partial \phi_x}{\partial x} = - \frac{\partial \phi_y}{\partial y}$$

will be identically satisfied if a function ϕ exists such that

$$\begin{aligned} \phi_x &= - \frac{\partial \phi}{\partial y} \\ \phi_y &= \frac{\partial \phi}{\partial x} \, . \end{aligned} \tag{3.72}$$

Substituting the equations (3.72) into (3.14) gives

$$\sigma_x = - \frac{\partial}{\partial y}\left(- \frac{\partial \phi}{\partial y}\right) = \frac{\partial^2 \phi}{\partial y^2}$$

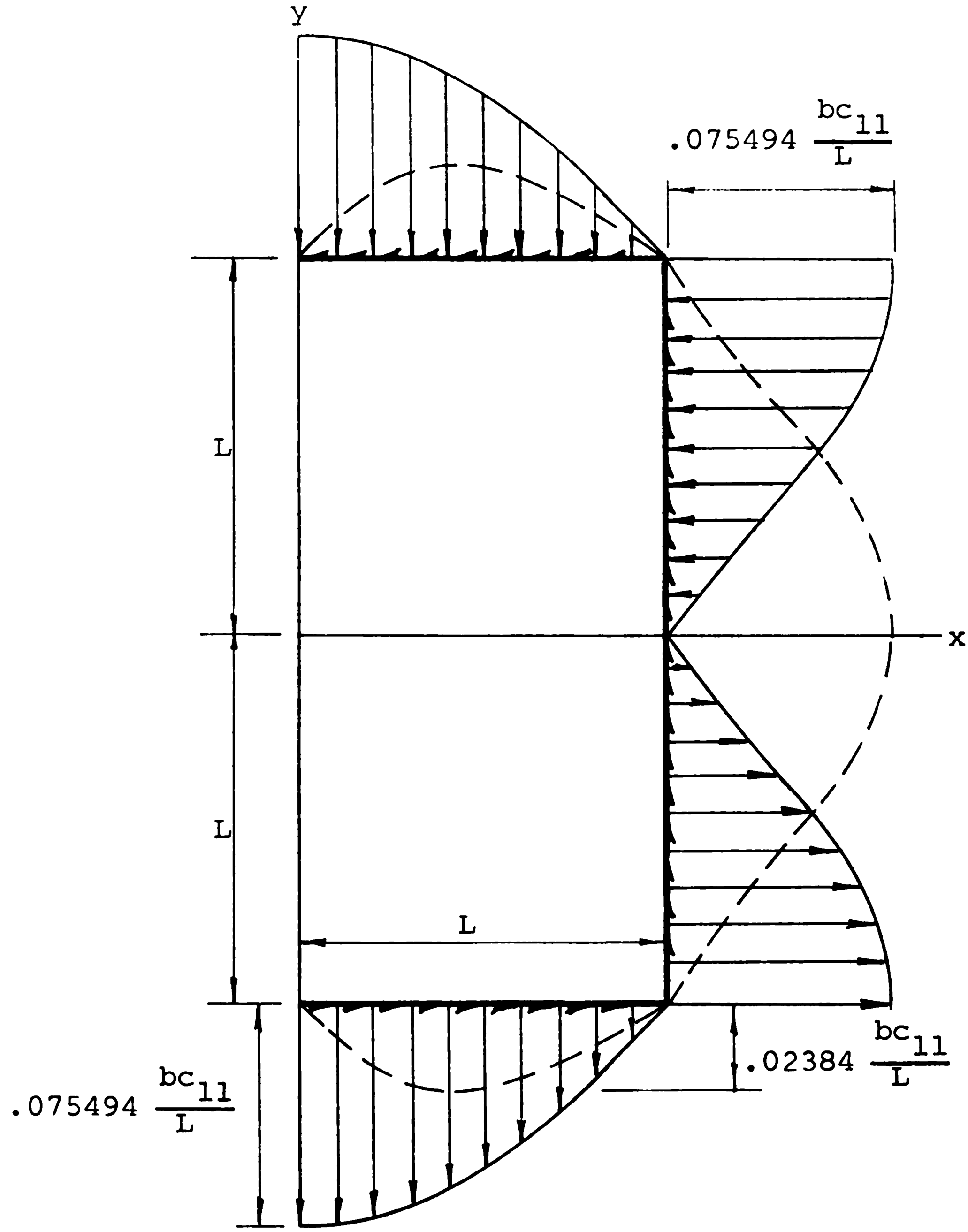


Fig. 12.--Boundary stresses for finite difference solution

$$\tau_{xy} = \frac{\partial}{\partial x}\left(-\frac{\partial \phi}{\partial y}\right) = -\frac{\partial}{\partial y}\left(\frac{\partial \phi}{\partial x}\right) = -\frac{\partial^2 \phi}{\partial x \partial y} \tag{3.73}$$

$$\sigma_y = \frac{\partial}{\partial x}\left(\frac{\partial \phi}{\partial x}\right) = \frac{\partial^2 \phi}{\partial x^2}.$$

It is shown in Appendix V that the function ϕ, for the case of cubic anisotropy must satisfy the compatibility equation

$$c_{11}\frac{\partial^4 \phi}{\partial x^4} + \frac{c_{11}{}^2 - 2c_{12}c_{44} - c_{12}{}^2}{c_{44}} \frac{\partial^4 \phi}{\partial x^2 \partial y^2} + c_{11}\frac{\partial^4 \phi}{\partial y^4} = 0 \tag{3.74}$$

which for the special case $c_{12} = c_{44} = c_{11}/2$ becomes

$$\frac{\partial^4 \phi}{\partial x^4} + \frac{1}{2}\frac{\partial^4 \phi}{\partial x^2 \partial y^2} + \frac{\partial^4 \phi}{\partial y^4} = 0. \tag{3.75}$$

Note that if the relationship

$$c_{44} = \tfrac{1}{2}(c_{11} - c_{12})$$

which holds for isotropic materials is substituted into equation (3.75) the biharmonic compatibility equation of isotropic elasticity is the result.

The boundary values of the function ϕ may be found by integration of the boundary stresses given by equations (3.66) through (3.71). This integration is carried out in Appendix VI. The boundary values of the stress function ϕ and its normal derivatives which result from this integration are given by the following equations. On the boundary $y_1 = 1$

$$\frac{\partial \phi}{\partial y_1} = bL \left[C_2 \frac{(1 + .5D)}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2x_1^{\,2} + D}{(4 - D^2)^{1/2}} - .25C_2 \log (x_1^{\,4} + Dx_1^{\,2} + 1) \right] \tag{3.76}$$

$$\phi = bL \left[\frac{.25C_2}{\cos\eta} x_1 \log \frac{x_1^{\,2} - 2x_1 \cos\eta + 1}{x_1^{\,2} + 2x_1 \cos\eta + 1} - .25C_2 \log (x_1^{\,4} + Dx_1^{\,2} + 1) + C_2 \frac{(1 + .5D)}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2x_1^{\,2} + D}{(4 - D^2)^{1/2}} \right] . \tag{3.77}$$

On the boundary $x_1 = 1$

$$\frac{\partial \phi}{\partial x_1} = bL \left[\frac{.25C_2}{\cos\eta} \log \frac{y_1^{\,2} - 2y_1 \cos\eta + 1}{y_1^{\,2} + 2y_1 \cos\eta + 1} \right] \tag{3.78}$$

$$\phi = bL \left[- \frac{C_1 - .5DC_2}{(4 - D^2)^{1/2}} y_1 \tan^{-1} \frac{2y_1^{\,2} + D}{(4 - D^2)^{1/2}} - .25C_2 y_1 \log (y_1^{\,4} + Dy_1^{\,2} + 1) + \frac{(DC_2 - C_1 - C_2)}{8 \cos\eta} \log \frac{y_1^{\,2} + 2y_1 \cos\eta + 1}{y_1^{\,2} - 2y_1 \cos\eta + 1} - \frac{(C_2 + C_2 D - C_1)}{4 \sin\eta} \tan^{-1} \frac{2y_1 \sin\eta}{1 - y_1^{\,2}} + \left(C_2 + \frac{C_1 + C_2}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2 + D}{(4 - D^2)^{1/2}} \right) y_1 + \frac{C_2 + DC_2 - C_1}{8 \cos\eta} \log \frac{1 - \cos\eta}{1 + \cos\eta} + \frac{(C_2 + C_2 D - C_1)\pi}{8 \sin\eta} - C_2 \right] \tag{3.79}$$

On the boundary $y_1 = -1$

$$\frac{\partial\phi}{\partial y_1} = bL\left[C_2 \frac{(1 + .5D)}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2x_1^{\,2} + D}{(4 - D^2)^{1/2}} - \right.$$

$$\left. .25C_2 \log (x_1^{\,4} + Dx_1^{\,2} + 1)\right] \qquad (3.80)$$

$$\phi = bL\left[\frac{-.25C_2}{\cos\eta} x_1 \log \frac{x_1^{\,2} - 2x_1 \cos\eta + 1}{x_1^{\,2} + 2x_1 \cos\eta + 1} + \right.$$

$$.25C_2 \log (x_1^{\,4} + Dx_1^{\,2} + 1) - C_2 \frac{(1 + .5D)}{(4 - D^2)^{1/2}} \tan^{-1}$$

$$\frac{2x_1^{\,2} + D}{(4 - D^2)^{1/2}} + \frac{C_2 + DC_2 - C_1}{4 \cos\eta} \log \frac{1 - \cos\eta}{1 + \cos\eta} +$$

$$\left.\frac{(C_2 + C_2D - C_1)\pi}{4 \sin\eta} - 2C_2\right] . \qquad (3.81)$$

Noting the impossibility of finding an analytic solution of equation (3.75) which will satisfy the conditions (3.76) through (3.81), a finite difference approximation will be made.

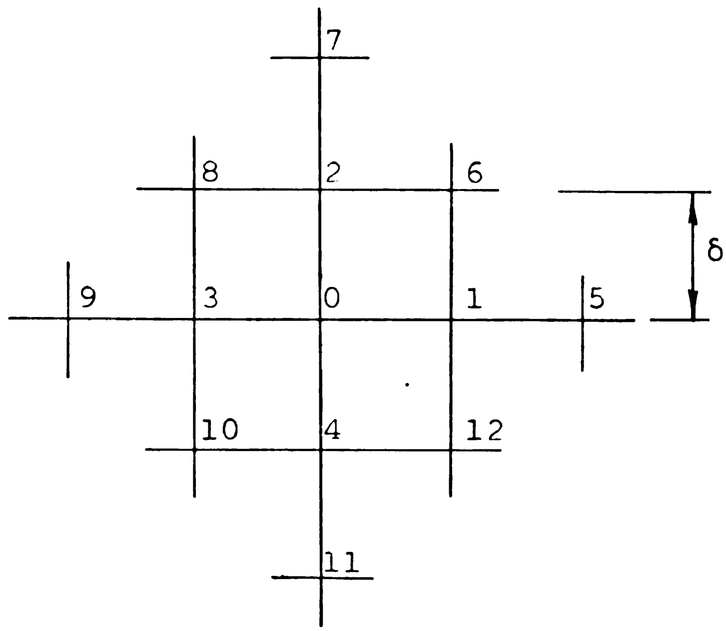
b) Finite Difference Approximation

The difference approximation of the equation (3.75), referring to Figure 13a, is

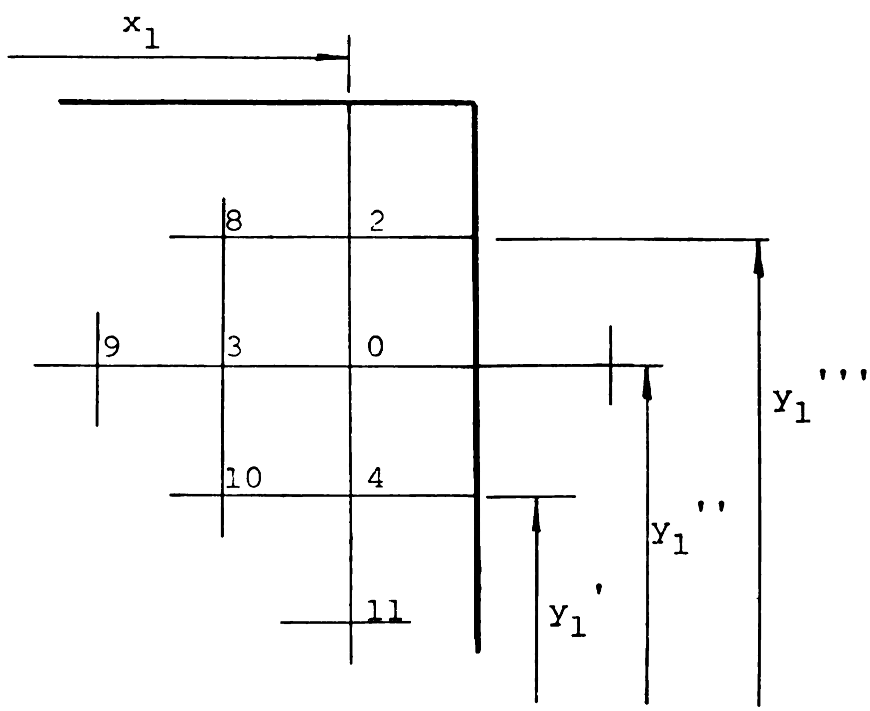
$$14\phi_0 - 5(\phi_1 + \phi_2 + \phi_3 + \phi_4) + (\phi_5 + \phi_7 + \phi_9 + \phi_{11}) +$$

$$.5(\phi_6 + \phi_8 + \phi_{10} + \phi_{12}) = 0. \qquad (3.82)$$

If the point 0 is one or two mesh spacings from a boundary, one or more of the points 0 through 12 fall on the boundary or one mesh spacing outside the boundary. The values of ϕ at points which fall on the boundary are evaluated directly from the equation (3.77), (3.79), or (3.81). The value of



(a)



(b)

Fig. 13.--Finite difference mesh for the approximation of the compatibility equation

at points which fall outside the boundary are, by the central difference approximation, assumed to equal the unknown value of ϕ at the adjacent interior mesh point plus the product of the normal derivative at the boundary as given by equation (3.76), (3.78), or (3.80) and twice the mesh spacing δ. On the lower boundary the sign of δ is negative since y_1 is positive in the upward direction.

Referring to Figure 13b, where point 0 is one mesh spacing from the side boundary and two from the top boundary, the finite difference equation (3.82) at 0 is

$$14\phi_0 - 5[\phi(y_1'') + \phi_2 + \phi_3 + \phi_4] + \phi_0 + 2\delta \frac{\partial \phi(y_1'')}{\partial x_1} + \phi(x_1) + \phi_9 + \phi_{11} + .5[\phi(y_1''') + \phi_8 + \phi_{10} + \phi(y_1')] = 0. \tag{3.83}$$

Collecting the known quantities on the right hand side gives

$$15\phi_0 - 5(\phi_2 + \phi_3 + \phi_4) + \phi_9 + \phi_{11} + .5(\phi_8 + \phi_{10}) = 5\phi(y_1'') - 2\delta \frac{\partial \phi(y_1'')}{\partial x_1} - \phi(x_1) - .5\,[\phi(y_1''') + \phi(y_1')]. \tag{3.84}$$

The set of finite difference equations for the mesh of Figure 14 with $\delta = .125$ is given in Appendix V. This system may be most easily solved by a Seidel iteration. After 8,000 cycles, with an initial solution vector of zero, the greatest change in any of the 120 unknown values

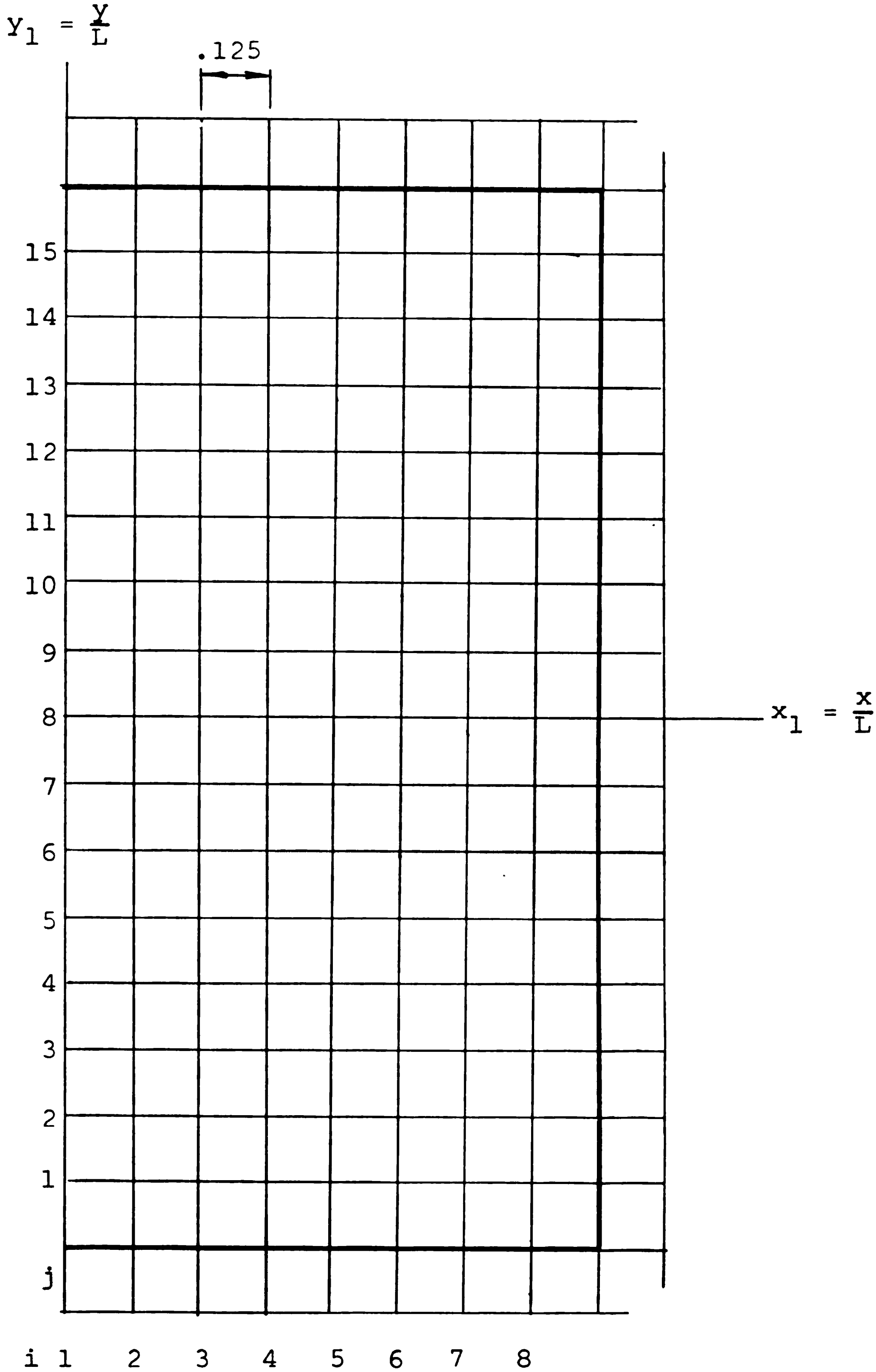


Fig. 14.--Mesh for numerical solution

of ϕ due to the last iteration was 1.82×10^{-12}. This was believed to be sufficiently small to define convergence. The running time on the CDC 3600 computer for the program which determined ϕ and also stresses and displacements in the region was 4 minutes and 55 seconds. This Fortran program may be found in Appendix VIII. Values of the stress function at interior, boundary, and exterior points are shown in Table 9.

It should be noted that a direct solution of this system of equations, which involves 120 members, is possible on the CDC 3600 if the quasi-diagonal property of the coefficient matrix is taken into account. (If the entire coefficient matrix including all zero values is input, the available computer memory is exceeded.) Because of the questionable accuracy of the direct solution, due to loss of significant figures, and because of the programing difficulties involved, the iteration method was used instead. A direct solution was determined for a mesh of 28 interior points. When single precision arithmetic (12 significant figures) was used, large errors appeared in the solution. However, a double precision arithmetic (24 significant figures) solution agreed exactly with an iterated solution, both having errors on the order of 10^{-12}.

Values of stresses at the interior and boundary points were determined by the finite difference approximations of the second derivatives of ϕ. Referring to Figure 13a the equations from which the stresses at mesh point 0 were determined are

TABLE 9

STRESS FUNCTION FOR NUMERICAL SOLUTION (bc_{11}/L)

1.125	.0118160	.0113453	.0099474	.0076637	.0045595	.0007223	-.0037372	-.0086887	-.0139962	
1.	.0123134	.0117259	.0099912	.0071928	.0034683	-.0009988	-.0059994	-.0113253	-.0167953	-.0223082
.875	.0087377	.0081212	.0063070	.0033990	-.0004370	-.0049900	-.0100320	-.0153512	-.0207804	-.0262012
.750	.0019057	.0013209	-.0003973	-.0031439	-.0067561	-.0110346	-.0157725	-.0207878	-.0259486	-.0311807
.625	-.0074964	-.0080113	-.0095236	-.0119398	-.0151186	-.0188915	-.0230900	-.0275734	-.0322536	-.0371126
.500	-.0188935	-.0193169	-.0205606	-.0225497	-.0251720	-.0282974	-.0317997	-.0355799	-.0395879	-.0438386
.375	-.0317969	-.0321181	-.0330623	-.0345745	-.0365739	-.0389684	-.0416714	-.0446199	-.0477882	-.0511971
.250	-.0457817	-.0459966	-.0466285	-.0476421	-.0489860	-.0506025	-.0524393	-.0544601	-.0566528	-.0590304
.125	-.0604660	-.0605734	-.0608895	-.0613972	-.0620715	-.0628852	-.0638138	-.0648412	-.0659624	-.0671820
0	-.0754938	-.0754938	-.0754938	-.0754938	-.0754938	-.0754938	-.0754938	-.0754938	-.0754938	-.0754938
- .125	-.0905217	-.0904142	-.0900981	-.0895905	-.0889161	-.0881025	-.0871738	-.0861464	-.0850253	-.0838057
- .250	-.1052059	-.1049911	-.1043592	-.1033455	-.1020016	-.1003851	-.0985484	-.0965275	-.0943348	-.0919573
- .375	-.1191907	-.1188695	-.1179254	-.1164132	-.1144137	-.1120193	-.1093162	-.1063678	-.1031994	-.0997905
- .500	-.1320942	-.1316708	-.1304270	-.1284380	-.1258156	-.1226902	-.1191880	-.1154077	-.1113997	-.1071491
- .625	-.1434912	-.1429763	-.1414640	-.1390478	-.1358691	-.1320961	-.1278976	-.1234143	-.1187340	-.1138751
- .750	-.1528934	-.1523086	-.1505903	-.1478438	-.1442316	-.1399531	-.1352151	-.1301998	-.1250391	-.1198070
- .875	-.1597253	-.1591088	-.1572947	-.1543867	-.1505507	-.1459976	-.1409557	-.1356365	-.1302073	-.1247865
-1.	-.1633010	-.1627135	-.1609788	-.1581804	-.1544560	-.1499888	-.1449882	-.1396623	-.1341924	-.1286794
-1.125	-.1628036	-.1623329	-.1609350	-.1586513	-.1555471	-.1517099	-.1472504	-.1422989	-.1369914	
y_1 x_1	0	.125	.250	.375	.500	.625	.750	.875	1.000	1.125

$$(\sigma_x)_0 = \left(\frac{\partial^2\phi}{\partial y^2}\right)_0 \simeq \frac{\phi_2 - 2\phi_0 + \phi_4}{\delta^2}$$

$$(\sigma_y)_0 = \left(\frac{\partial^2\phi}{\partial x^2}\right)_0 \simeq \frac{\phi_1 - 2\phi_0 + \phi_3}{\delta^2} \tag{3.85}$$

$$(\tau_{xy})_0 = \left(-\frac{\partial^2\phi}{\partial x\,\partial y}\right)_0 \simeq \frac{\phi_6 + \phi_{10} - \phi_8 - \phi_{12}}{4\delta^2}.$$

The values of stresses are shown in Tables 10, 11, and 12. The variation of these stresses along various horizontal and vertical lines are graphically illustrated in Appendix IX.

c) Determination of Displacements

The displacements are related to the stress function by the equations

$$c_{11}\frac{\partial u}{\partial x} + c_{12}\frac{\partial v}{\partial y} = \frac{\partial^2\phi}{\partial y^2} \tag{3.86}$$

$$c_{11}\frac{\partial v}{\partial y} + c_{12}\frac{\partial u}{\partial x} = \frac{\partial^2\phi}{\partial x^2} \tag{3.87}$$

$$c_{44}\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) = -\frac{\partial^2\phi}{\partial x\,\partial y}. \tag{3.88}$$

Solving the equations (3.86) and (3.87) simultaneously for $\partial u/\partial x$ and $\partial v/\partial y$ leads to the values

$$\frac{\partial u}{\partial x} = \frac{c_{11}}{c_{11}^2 - c_{12}^2}\frac{\partial^2\phi}{\partial y^2} - \frac{c_{12}}{c_{11}^2 - c_{12}^2}\frac{\partial^2\phi}{\partial x^2} \tag{3.89}$$

$$\frac{\partial v}{\partial y} = \frac{c_{11}}{c_{11}^2 - c_{12}^2}\frac{\partial^2\phi}{\partial x^2} - \frac{c_{12}}{c_{11}^2 - c_{12}^2}\frac{\partial^2\phi}{\partial y^2}. \tag{3.90}$$

TABLE 10

σ_x FOR NUMERICAL SOLUTION (bc_{11}/L, σ_x IS ANTISYMMETRICAL WITH RESPECT TO $y_1 = 0$)

0	0	0	0	0	0	0	0	0	0
- .125	.02199	.02199	.02197	.02186	.02155	.02086	.01955	.01737	.01420
- .250	.04476	.04470	.04447	.04400	.04310	.04150	.03883	.03462	.02848
- .375	.06921	.06894	.06813	.06674	.06465	.06165	.05735	.05122	.04252
- .500	.09641	.09573	.09374	.09056	.08630	.08096	.07437	.06614	.05542
- .625	.12767	.12629	.12229	.11609	.10822	.09914	.08910	.07814	.06587
- .750	.16449	.16205	.15501	.14419	.13078	.11600	.10093	.08633	.07276
- .875	.20840	.20452	.19330	.17595	.15449	.13141	.10931	.09029	.07572
-1.	.26068	.25506	.23859	.21266	.18011	.14529	.11330	.08891	.07591
y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.

TABLE 11

σ_y FOR NUMERICAL SOLUTION (bc_{11}/L, σ_y IS ANTISYMMETRICAL WITH RESPECT TO $y_1 = 0$)

y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.
0	0	0	0	0	0	0	0	0	
− .125	.01375	.01336	.01226	.01067	.00891	.00736	.00633	.00600	.00630
− .250	.02750	.02669	.02443	.02114	.01745	.01409	.01178	.01100	.01183
− .375	.04111	.03987	.03635	.03118	.02528	.01975	.01570	.01407	.01540
− .500	.05420	.05250	.04770	.04053	.03220	.02412	.01779	.01458	.01553
− .625	.06591	.06383	.05785	.04880	.03803	.02723	.01823	.01260	.01144
− .750	.07486	.07254	.06581	.05540	.04264	.02940	.01775	.00931	.00457
− .875	.07891	.07665	.07000	.05939	.04589	.03129	.01774	.00704	.00054
−1.	.07520	.07342	.06808	.05926	.04753	.03414	.02082	.00922	0

TABLE 12

τ_{xy} FOR NUMERICAL SOLUTION (bc_{11}/L, τ_{xy} IS SYMMETRICAL WITH RESPECT TO $y_1 = 0$)

0	0	.01355	.02636	.03782	.04762	.05575	.06259	.06876	.07490
- .125	0	.01355	.02633	.03772	.04737	.05525	.06172	.06742	.07312
- .250	0	.01347	.02612	.03727	.04649	.05368	.05913	.06349	.06778
- .375	0	.01313	.02540	.03606	.04460	.05079	.05480	.05719	.05901
- .500	0	.01219	.02355	.03333	.04093	.04598	.04849	.04875	.04739
- .625	0	.01017	.01971	.02796	.03429	.03822	.03953	.03821	.03415
- .750	0	.00645	.01270	.01838	.02300	.02598	.02687	.02535	.02097
- .875	0	.00031	.00109	.00263	.00481	.00722	.00917	.00992	.00920
-1.	0	-.00899	-.01665	-.02170	-.02316	-.02077	-.01520	-.00783	
y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.

For the case of $c_{12} = c_{44} = \frac{c_{11}}{2}$ and after making the substitutions $x_1 = x/L$, $y_1 = y/L$ these equations become

$$\frac{\partial u}{\partial x_1} = \frac{4}{3c_{11}L}\left(\frac{\partial^2\phi}{\partial y_1^2} - .5\frac{\partial^2\phi}{\partial x_1^2}\right) \tag{3.91}$$

$$\frac{\partial v}{\partial y_1} = \frac{4}{3c_{11}L}\left(\frac{\partial^2\phi}{\partial x_1^2} - .5\frac{\partial^2\phi}{\partial y_1^2}\right). \tag{3.92}$$

Consider the finite difference form of the equation (3.91) for the lattice point i = 1,j of Figure 14. This point lies on the y_1 axis j mesh spacings above the lower boundary. Using a central difference approximation for all derivatives and noting that because of symmetry

$$u(0,y_1) = 0$$

$$u(-x_1,y_1) = -u(x_1,y_1)$$

$$\phi(-x_1,y_1) = \phi(x_1,y_1)$$

the finite difference approximation of equation (3.91) at this point is

$$\frac{u_{2,j} - (-u_{2,j})}{2\delta} = \frac{4}{3c_{11}L}\quad\frac{(\phi_{1,j+1} - 2\phi_{1,j} + \phi_{1,j-1})}{\delta^2} -$$
$$.5\,\frac{(\phi_{2,j} - 2\phi_{1,j} + \phi_{2,j})}{\delta^2} \quad .$$

Simplifying this equation gives

$$u_{2,j} = \frac{8}{3c_{11}L\delta}\left[\phi_{1,j+1} + \phi_{1,j-1} - \phi_{2,j} - \phi_{1,j}\right]. \tag{3.93}$$

The finite difference equation at the point i = 2,j is

$$\frac{u_{3,j} - u_{1,j}}{2\delta} = \frac{4}{3c_{11}L}\left[\frac{(\phi_{2,j+1} - 2\phi_{2,j} + \phi_{2,j-1})}{\delta^2} - .5(\phi_{3,j} - 2\phi_{2,j} + \phi_{1,j})\right].$$

Simplifying and noting that $u_{1,j} = 0$ because of symmetry gives

$$u_{3,j} = \frac{8}{3c_{11}\delta L}[\phi_{2,j+1} + \phi_{2,j-1} - .5\phi_{3,j} - .5\phi_{1,j} - \phi_{2,j}]. \tag{3.94}$$

For the point i,j the finite difference equation is

$$u_{i+1,j} = \frac{8}{3c_{11}\delta L}[\phi_{i,j+1} + \phi_{i,j-1} - .5\phi_{i+1,j} - .5\phi_{i-1,j} - \phi_{i,j}] + u_{i-1,j}. \tag{3.95}$$

Using the equation (3.95) at successive points on the horizontal mesh line allows the calculation of all u displacements on that line. Use of the equations (3.93) through (3.95) on every horizontal mesh line will yield u displacements at all mesh points in the region. Values of u for the mesh shown in Figure 14 appear in Table 13.

It is known that the value of the v displacement at the point (0,-1) in the x_1, y_1 plane is zero.

$$v(0,-1) = 0$$

If the central difference approximation of equation (3.92) is written for the mesh point i = 1, j = 1 the result is the following:

TABLE 13

u DISPLACEMENTS FOR NUMERICAL SOLUTION (b, u IS ANTISYMMETRICAL WITH RESPECT TO $y_1 = 0$)

0	0	0	0	0	0	0	0	0	0
-.125	0	.00252	.00510	.00780	.01061	.01350	.01634	.01896	.02113
-.250	0	.00517	.01045	.01592	.02159	.02738	.03308	.03836	.04278
-.375	0	.00811	.01634	.02476	.03338	.04210	.05064	.05860	.06537
-.500	0	.01155	.02316	.03485	.04659	.05825	.06956	.08007	.08918
-.625	0	.01578	.03146	.04691	.06202	.07664	.09053	.10330	.11448
-.750	0	.02118	.04193	.06188	.08076	.09836	.11452	.12905	.14174
-.875	0	.02816	.05540	.08092	.10415	.12477	.14274	.15825	.17166
-1.	0	.03718	.07278	.10536	.13379	.15748	.17653	.19177	.20463
y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.

$$\frac{v_{1,2} - v(0,-1)}{2\delta} = \frac{4}{3c_{11}L} \frac{(\phi_{2,2} - 2\phi_{1,2} + \phi_{2,2})}{\delta^2} - .5\frac{(\phi_{1,3} - 2\phi_{1,2} + \phi_{1,1})}{\delta^2} .$$

Since $v(0,-1) = 0$ this simplifies to

$$v_{1,2} = \frac{8}{3c_{11}L\delta} [2\phi_{2,2} - .5\phi_{1,3} - .5\phi_{1,1} - \phi_{1,2}]. \tag{3.96}$$

The difference equation at point $i = 1,j$ where j is an odd integer is

$$v_{1,j+1} = \frac{8}{3c_{11}L\delta} [2\phi_{2,j} - .5\phi_{1,j+1} - .5\phi_{1,j-1} - \phi_{1,j}] + v_{1,j-1}. \tag{3.97}$$

Successive use of this equation for all even values of j will give the v displacements at all mesh points on the y_1 axis for which j is even.

The finite difference form of equation (3.88) for the point i,j for the case $c_{44} = c_{11}/2$ is

$$\frac{c_{11}}{2}\left(\frac{v_{i+1,j} - v_{i-1,j}}{2\delta} + \frac{u_{i,j+1} - u_{i,j-1}}{2\delta}\right) = -\frac{1}{L}\left(\frac{\phi_{i+1,j+1} + \phi_{i-1,j-1} - \phi_{i+1,j-1} - \phi_{i-1,j+1}}{4\delta^2}\right).$$

Solving for $v_{i+1,j}$ gives the equation

$$v_{i+1,j} = \frac{1}{c_{11}L\delta} (\phi_{i+1,j+1} + \phi_{i-1,j-1} - \phi_{i+1,j-1} - \phi_{i-1,j+1}) + v_{i-1,j} - u_{i,j+1} + u_{i,j-1}. \tag{3.98}$$

Since $v_{1,j}$ is known for all even values of j and all values of u have been previously calculated, the equation (3.98) may be written for the point i = 2,j and the displacement $v_{3,j}$ immediately determined. Similarly, the value of $v_{i,j}$ for all odd values of i may be determined on every horizontal mesh line for which j is even. The v displacements, then, may be determined at mesh points at which i is odd and j is even by using equations (3.97) and (3.98). The values of v for the mesh of Figure 14 are shown in Table 14, and graphical representations of u and v appear in Appendix IX.

The results of the analytic solution shown in Tables 4 through 8 may now be added to the results of the numerical solution shown in Tables 9 through 14. The superimposed solution is shown in Tables 15 through 19 and will henceforth be referred to as the combined continuum solution.

d) An Alternative Method for Finding Displacements

An alternative method, which is theoretically more accurate than the one just described, may be used to determine displacements. This method involves the integrated forms of equations (3.88), (3.89), and (3.90).

The u displacement is determined by integrating equation (3.89) from x_0 to x

$$u(x) - u(x_0) = \frac{c_{11}}{c_{11}^2 - c_{12}^2} \int_{x_0}^{x} \frac{\partial^2 \phi}{\partial y^2}\, dx - \frac{c_{12}}{c_{11}^2 - c_{12}^2} \left[\frac{\partial \phi(x)}{\partial x} - \frac{\partial \phi(x_0)}{\partial x}\right]. \tag{3.99}$$

TABLE 14

v DISPLACEMENTS FOR NUMERICAL SOLUTION (b, v IS SYMMETRICAL WITH RESPECT TO y_1 = 0)

y_1 \ x_1	0	.25	.50	.75	1.
0	-.00465	.00716	.04167	.09655	.16885
- .25	-.00557	.00676	.04235	.09779	.16917
- .50	-.00739	.00603	.04485	.10239	.17147
- .75	-.00843	.00717	.05037	.11148	.17910
-1.	0	.01605	.06082	.12379	.19190

TABLE 15

u DISPLACEMENT FOR COMBINED CONTINUUM SOLUTION (b)

1.	0	-.03077	-.05931	-.08361	-.10223	-.11461	-.12123	-.12352	-.12356
.875	0	-.02080	-.03971	-.05516	-.06629	-.07310	-.07635	-.07718	-.07671
.750	0	-.01252	-.02310	-.03032	-.03384	-.03444	-.03345	-.03189	-.03019
.625	0	-.00525	-.00787	-.00641	-.00156	.00443	.00965	.01350	.01634
.500	0	.00192	.00840	.02045	.03448	.04634	.05456	.05973	.06319
.375	0	.01072	.02958	.05631	.07817	.09286	.10173	.10689	.11026
.250	0	.02639	.07062	.11820	.13078	.14349	.15057	.15458	.15719
.125	0	.07855	.14727	.17585	.18936	.19638	.20019	.20233	.20374
0	0	.25000	.25000	.25000	.25000	.25000	.25000	.25000	.25000
- .125	.50000	.42145	.35273	.32415	.31064	.30362	.29981	.29767	.29626
- .250	.50000	.47361	.42948	.39180	.36922	.35651	.34943	.34542	.34281
- .375	.50000	.48928	.46942	.44369	.42183	.40714	.39827	.39311	.38974
- .500	.50000	.49808	.49160	.47955	.46552	.45366	.44544	.44027	.43681
- .625	.50000	.50525	.50787	.50641	.50156	.49557	.49035	.48650	.48366
- .750	.50000	.51252	.52310	.53032	.53084	.53444	.53345	.53189	.53619
- .875	.50000	.52080	.53846	.55516	.56629	.57310	.57635	.57718	.57671
-1.	.50000	.53078	.55931	.58361	.60223	.61461	.62350	.62352	.62356
y_1 / x_1	0	.125	.250	.375	.500	.625	.750	.875	1.

TABLE 16

v DISPLACEMENTS FOR COMBINED CONTINUUM SOLUTION (b, v IS SYMMETRICAL WITH RESPECT TO y_1 = 0)

0	-	.06576	.13525	.21054	.29732
- .25	-.07534	.01275	.11626	.20243	.29227
- .50	-.04328	-.00486	.08573	.18477	.28027
- .75	-.02291	.00368	.07631	.17276	.26204
-1.	0	.02229	.08481	.17310	.26766
y_1 / x_1	0	.25	.50	.75	1.

TABLE 17

σ_x FOR COMBINED SOLUTION (bc_{11}/L, σ_x IS ANTISYMMETRICAL WITH RESPECT TO $y_1 = 0$)

y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.
0	-	0	0	0	0	0	0	0	0
- .125	-.58196	-.58196	-.20054	-.07938	-.03543	-.01556	-.00571	-.00117	.00001
- .250	-.25722	-.30496	-.25751	-.13981	-.06815	-.03104	-.01179	-.00260	-.00001
- .375	-.13211	-.15100	-.16820	-.13458	-.08154	-.04128	-.01682	-.00409	-.00009
- .500	-.05458	-.06380	-.08109	-.08368	-.06469	-.03860	-.01754	-.00477	-.00021
- .625	.00688	.00096	-.01318	-.02595	-.02866	-.02165	-.01152	-.00361	-.00031
- .750	.06383	.05871	.04504	.03060	.01262	.00367	.00028	-.00033	-.00033
- .875	.12212	.11653	.10085	.07818	.05327	.03090	.01421	.00401	-.00029
-1.	.18519	.16194	.15882	.12880	.09270	.05646	.02618	.00654	.00042

TABLE 18

σ_y FOR COMBINED SOLUTION (bc_{11}/L, σ_y IS ANTISYMMETRICAL WITH RESPECT TO $y_1 = 0$)

y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.
0	-	0	0	0	0	0	0	0	
- .125	-.47020	.01336	.10762	.06653	.04310	.03006	.02240	.01795	.01552
- .250	-.27448	-.16403	.02443	.07366	.06513	.05080	.03971	.03261	.02892
- .375	-.16021	-.12870	-.04243	.03118	.05629	.05517	.04749	.04089	.03770
- .500	-.09679	-.08424	-.04766	-.00082	.03220	.04423	.04405	.04073	.03937
- .625	-.05488	-.04968	-.03392	-.01123	.01289	.02723	.03224	.03252	.03277
- .750	-.02580	-.02391	-.01798	-.00817	.00325	.01259	.01775	.01960	.02007
- .875	-.00737	-.00697	-.00564	-.00318	.00013	.00340	.00574	.00704	.00732
-1.	-.00029	-.00030	-.00029	-.00026	-.00015	.00001	.00015	.00023	

TABLE 19

τ_{xy} FOR COMBINED SOLUTION (bc_{11}/L, τ_{xy} IS SYMMETRICAL WITH RESPECT TO $y_1 = 0$)

y_1 \ x_1	0	.125	.250	.375	.500	.625	.750	.875	1.
0	-	-.59040	-.27562	-.16350	-.10337	-.06504	-.03807	-.01752	.00041
- .125	0	.01355	-.16439	-.12985	-.08937	-.05826	-.03473	-.01621	-.00060
- .250	0	.10883	.02612	-.04151	-.04887	-.03809	-.02466	-.01215	-.00059
- .375	0	.06899	.07792	.03606	.00325	-.00824	-.00877	-.00538	-.00051
- .500	0	.04638	.07123	.06434	.04093	.02084	-.00910	.00299	-.00029
- .625	0	.03287	.05642	.06338	.05440	.03822	.02272	.01032	.00002
- .750	0	.02252	.04063	.05017	.04926	.03999	.02687	.01335	.00030
- .875	0	.01226	.02270	.02945	.03096	.02714	.01946	.00992	.00021
-1.	0	.00023	.00044	.00062	.00068	.00056	.00030	.00003	0

For the particular problem considered here it is convenient to take x_0 as equal to zero. Then, by the displacement boundary condition and symmetry

$$u(x_0) = 0$$

$$\frac{\partial \phi(x_0)}{\partial x} = 0$$

for all y so that

$$u(x) = \frac{c_{11}}{c_{11}^2 - c_{12}^2} \int_0^x \frac{\partial^2 \phi}{\partial y^2} dx - \frac{c_{12}}{c_{11}^2 - c_{12}^2} \frac{\partial \phi(x)}{\partial x}. \tag{3.100}$$

The quantity $\frac{\partial \phi(x)}{\partial x}$ may be approximated by the first difference of ϕ. The values of $\frac{\partial^2 \phi}{\partial y^2}$ at all mesh points between 0 and x may be approximated by the second difference of ϕ at the various points and then numerically integrated over the interval. If a trapezoidal integration is used, u may be found at every mesh point or if the two-strip Simpson's parabolic integration is used, u may be found at every other mesh point. It is also possible to use a one-strip Simpson's rule in which the parabolas which approximate $(\Delta^2 \phi)_y$ overlap. In this case u may be found at every mesh point. The second term in equation (3.100) is evaluated at the point at which u is desired. This is clearly an advantage over the method of Section 3.3c since in that method the u value at each mesh point depended on the u value at the preceding mesh point allowing a possible accumulation of errors. Another possible increase in accuracy appears in the first term of equation (3.100) since the numerical integration of

$(\Delta^2\phi)_y$ will probably be a better approximation of $\int_0^x \frac{\partial^2\phi}{\partial y^2}dx$ than the values $(\Delta^2\phi)_y$ are of $\frac{\partial^2\phi}{\partial y^2}$.

The v displacements on the y axis may be found by an integration of equation (3.90) from point (0,-L), at which v = 0 to (0,y).

$$v(y) = \frac{c_{11}}{c_{11}^2 - c_{12}^2}\int_{-L}^{y} \frac{\partial^2\phi}{\partial x^2}dy - \frac{c_{12}}{c_{11}^2 - c_{12}^2}\left[\frac{\partial\phi(y)}{\partial y} - \frac{\partial\phi(-L)}{\partial y}\right]. \tag{3.101}$$

After having found the values of v on x = 0 equation (3.88) may be rearranged in the form

$$\frac{\partial v}{\partial x} = -\frac{1}{c_{44}}\frac{\partial^2\phi}{\partial x\partial y} - \frac{\partial u}{\partial y}.$$

Integrating this equation from 0 to x gives

$$v(x) - v(0) = -\frac{1}{c_{44}}\left[\frac{\partial\phi(x)}{\partial y} - \frac{\partial\phi(0)}{\partial y}\right] - \int_0^x \frac{\partial u}{\partial y}dx. \tag{3.102}$$

The calculation of several values of u using equation (3.100) and a Simpson's two strip integration gave values about 2% higher than the u's determined by the method of Section 3.3c. Since this difference is relatively small, no attempt was made to recalculate displacements using the more accurate method.

IV. DISCUSSION OF RESULTS

4.1. Results of the Discrete Analysis

The variation of u on various vertical atom planes defined by i = const is shown in Figure 15. Note that the values of u in this figure and for all succeeding figures of this section are for the right half of the lattice. This is for purposes of comparison with the continuum analysis which applies to the right half crystal. For this reason u values in these figures are opposite in sign to the values calculated by the system of equations in Appendix I and displayed in Table 1. The index i = 18 still corresponds to the extra atom plane and i = 1 still corresponds to the side boundary, however, in this case the right rather than the left side boundary.

Considering the atom plane immediately adjacent to the extra atom plane for which index i = 17, the u displacements of lattice points below the slip plane, j = 17, deviate only slightly from a value of .58b while those above the slip plane differ very little from zero. Most of the transition from .58b to 0 occurs between the three lattice points j = 16, 17, and 18. The relative u displacements between j = 16 and 17 and between

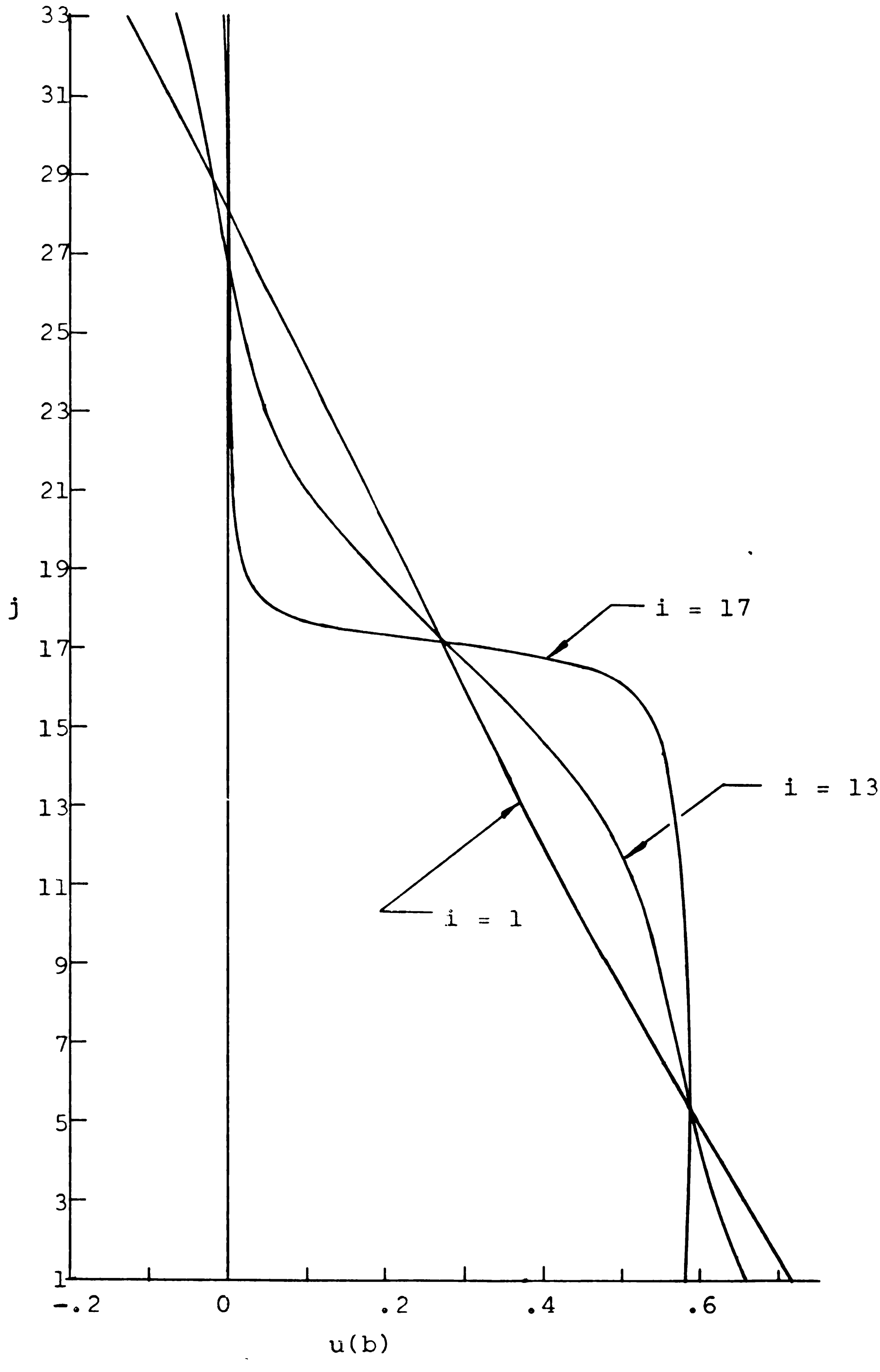


Fig. 15.--u displacement for discrete case versus j

j = 17 and 18 are .1774b and .2690b respectively. These large relative displacements are quickly distributed. On the vertical atom plane with index i = 13 the largest relative u displacement is approximately .05b. As the side boundary is approached the relative u displacement becomes more and more uniform until it becomes a virtually constant value of .025b at the boundary. The largest u displacement, .71b, occurs at the lower corner while the smallest algebraic value of u, -.122b, occurs at the upper corner.

An examination of Figure 16 which shows the variation of u on various horizontal atom planes defined by j = const also indicates that the region of large relative displacements is definitely limited to the region surrounding the lattice point i = 18, j = 17. Relative u displacements with values of .05b or greater occur only for certain pairs of lattice points lying in the region $17 \geq i \geq 14$, $21 \geq j \geq 14$. The antisymmetrical property of the u displacement is apparent after examining Figures 15 and 16. The value of u on the slip plane j = 17 is a nearly constant value of .27b and any two lattice points symmetrically located relative to the line j = 17 have approximately equal but opposite displacements relative to the displacement on the row j = 17.

The positive slope of a curve in Figure 16 indicates that the distance between two adjacent lattice points has increased and hence the mutual bond force is tensile. Similarly, a negative slope indicates a decrease

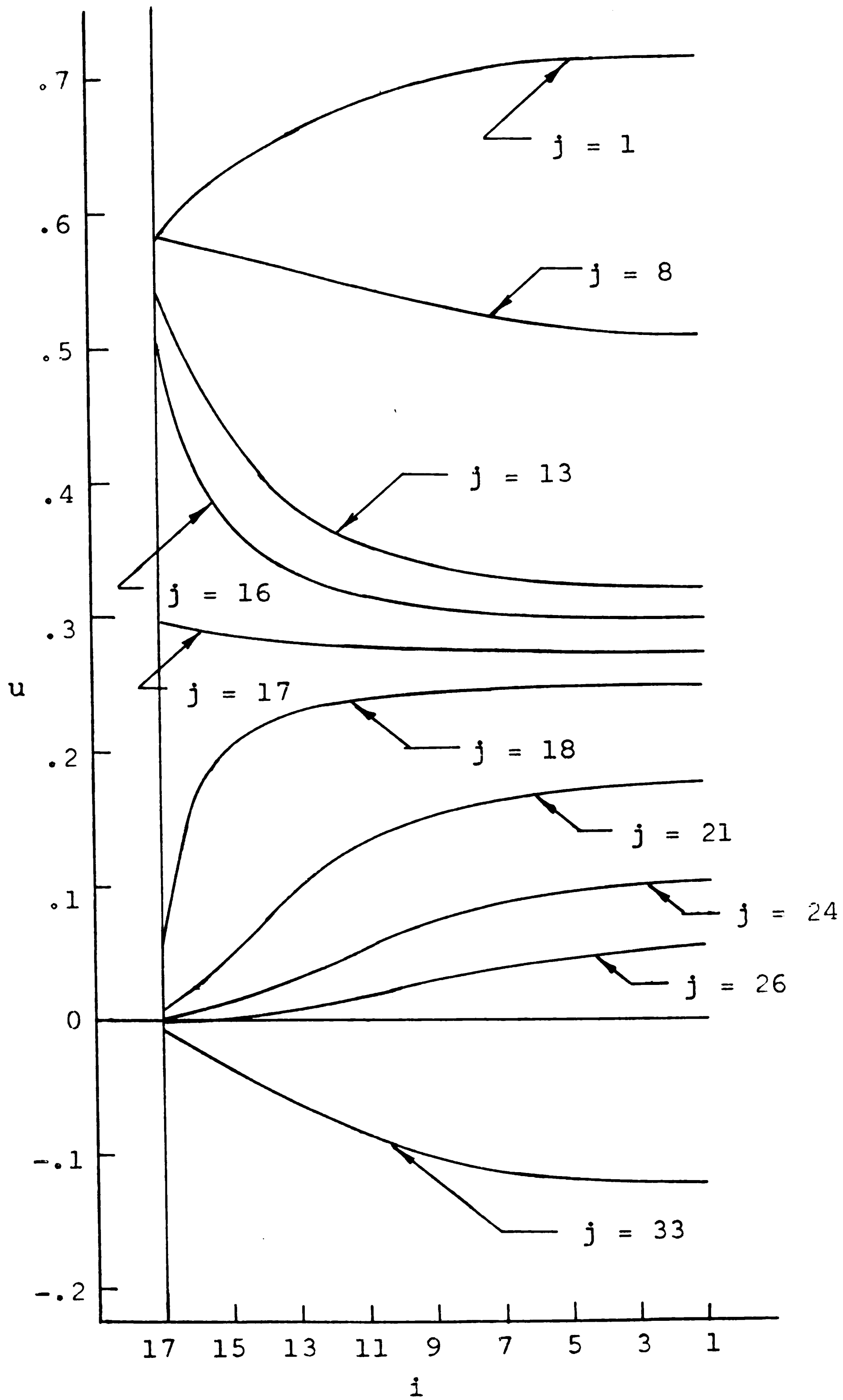


Fig. 16.--u displacement for discrete case versus i

in spacing and a compressive bond force. In the region adjacent to the lower boundary the lattice is in horizontal tension. Moving upward in the lattice a region of compression is encountered, followed by a region of tension and then a region of compression adjacent to the upper boundary. It may also be noted that for any constant j the slope is either always positive or always negative so that every row is either in tension or compression and never changes from one to another.

Figure 18 shows the variation of v along several horizontal atom planes. These curves indicate that from the vertical plane $i = 13$ to the side boundary v increases at an approximately constant slope for all values of j. In this region a horizontal plane of lattice points remains approximately straight but has been tilted upward, with $i = 18$ as the approximate pivot point. The general deformation of any particular horizontal row of lattice points involves an upward rotation of the row plus a varying tension or compression of the row. This tension or compression is maximum at $i = 17$ (next to the extra atom plane) and decreases in magnitude to zero at the side boundary. Most of the decrease takes place in the first four lattice spacings. A crude picture of the distorted lattice appears in Figure 21.

The general description of the deformed crystal lattice neglects some less important local variations. The most pronounced of these is the general increase in v as the horizontal lattice plane $j = 17$ is approached from

j less than 17 and the decrease as j becomes greater than 17. This characteristic is indicated by the bulge which appears in Figure 17 around the horizontal plane j = 17, and is most significant at the point (17,17) where the v displacements relative to lattice points (17,16) and (17,18) are .059b and -.062b respectively. This abrupt departure from the otherwise gradual variation of v may be explained by an examination of the bond forces acting on point (17,17) in Figure 8b. The vertical component of the force between point (17,17) and point (18,16) is not approximately cancelled by a symmetrically located point at (18,18) (since [18,18] does not exist). This vertical component, which is directed upward since the force is compressive, causes the increase in v. The magnitude of the relative v displacements associated with the bulge in Figure 17 decrease quickly and on the vertical lattice plane i = 14 the greatest relative vertical displacement is down to a value of .02b.

Distributions of lattice force components, F_x and F_{xy}, which act across vertical sections in the lattice are shown in Figures 19 and 20 for several different sections. Since there are no external forces acting on the lattice these distributions of force must be self-equilibrating. Summation of forces in the horizontal and vertical directions proved that the force resultant of the various distributions was zero since the resultants had a magnitude less than $10^{-7}\alpha b$. No calculations were made to determine resultant couples of the F_x distributions, but

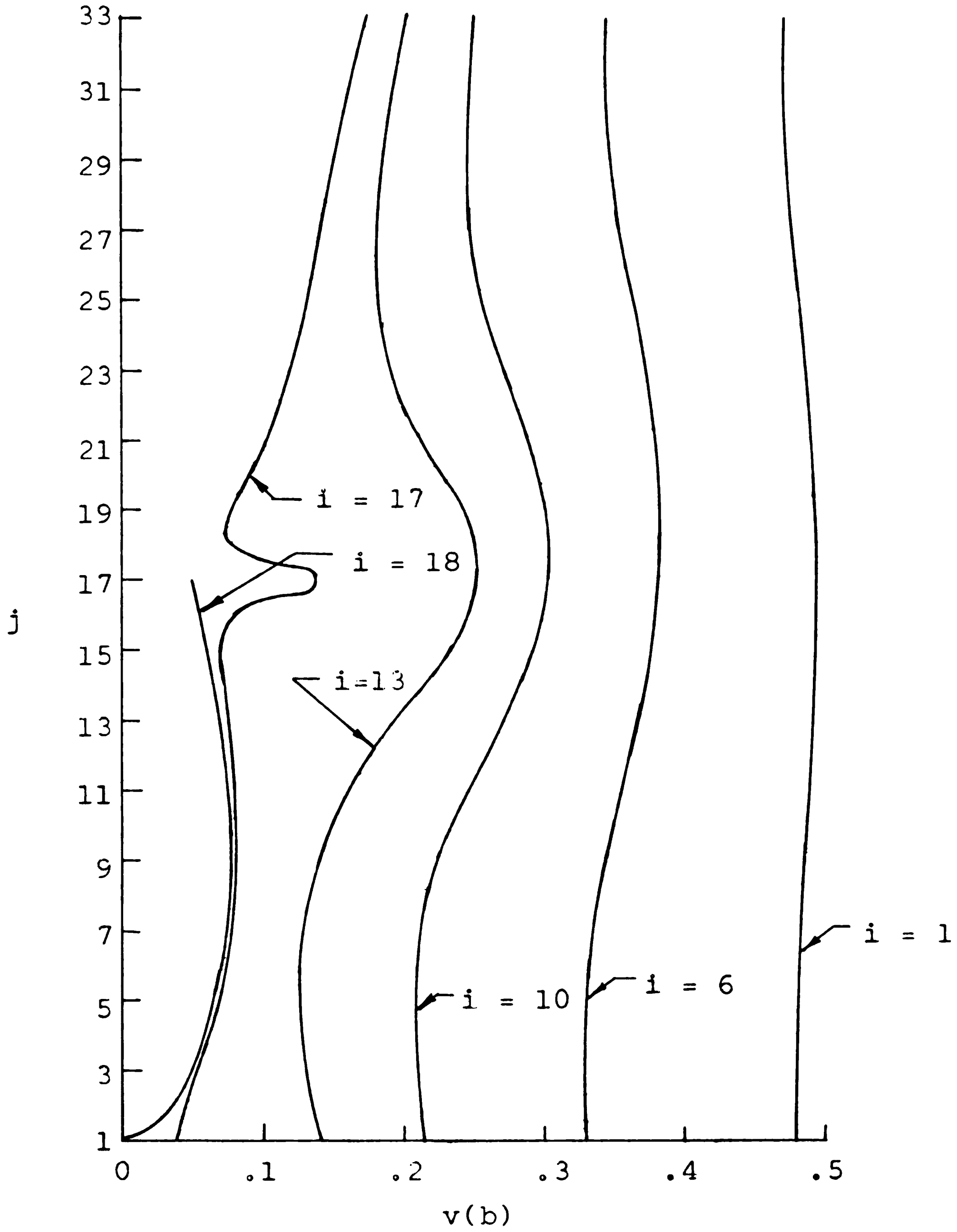


Fig. 17.--v displacement for discrete case versus j

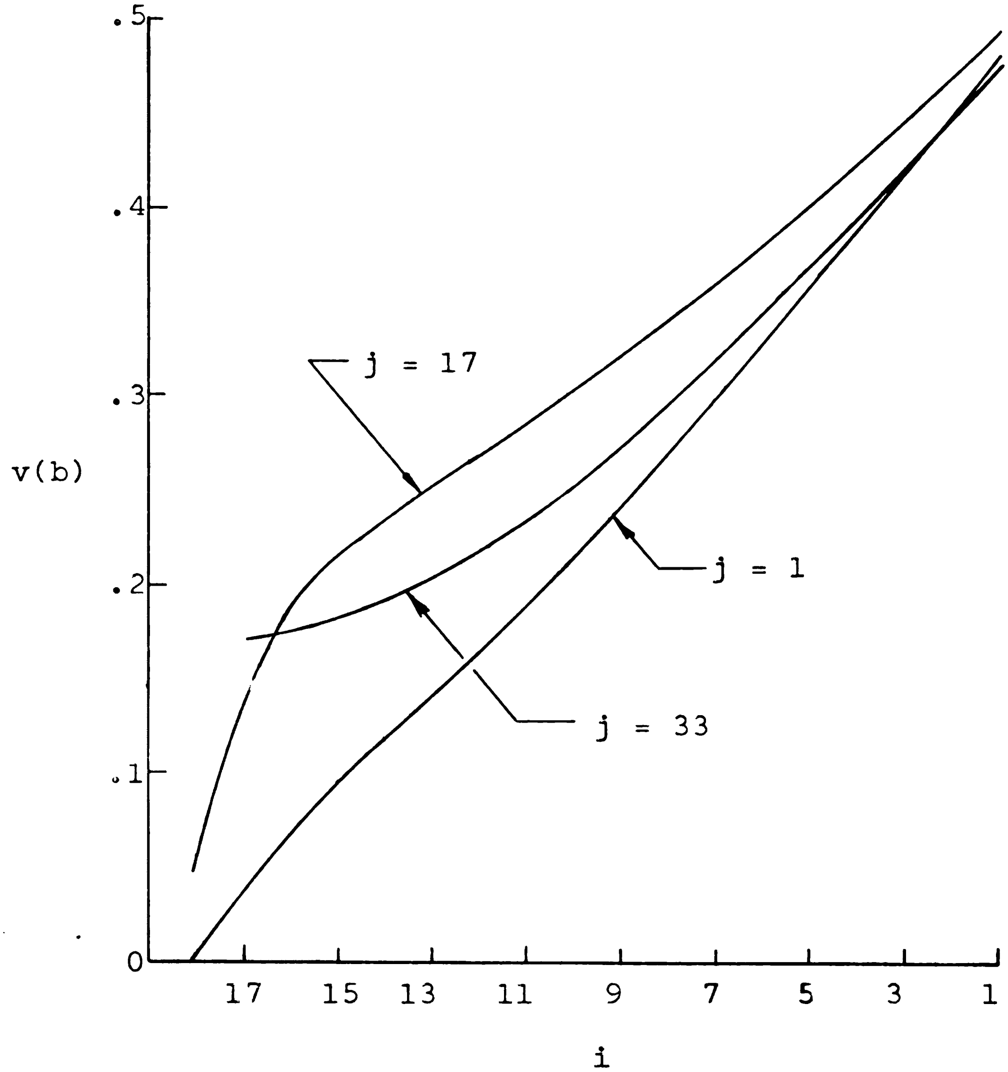


Fig. 18.--v displacement for discrete case versus i

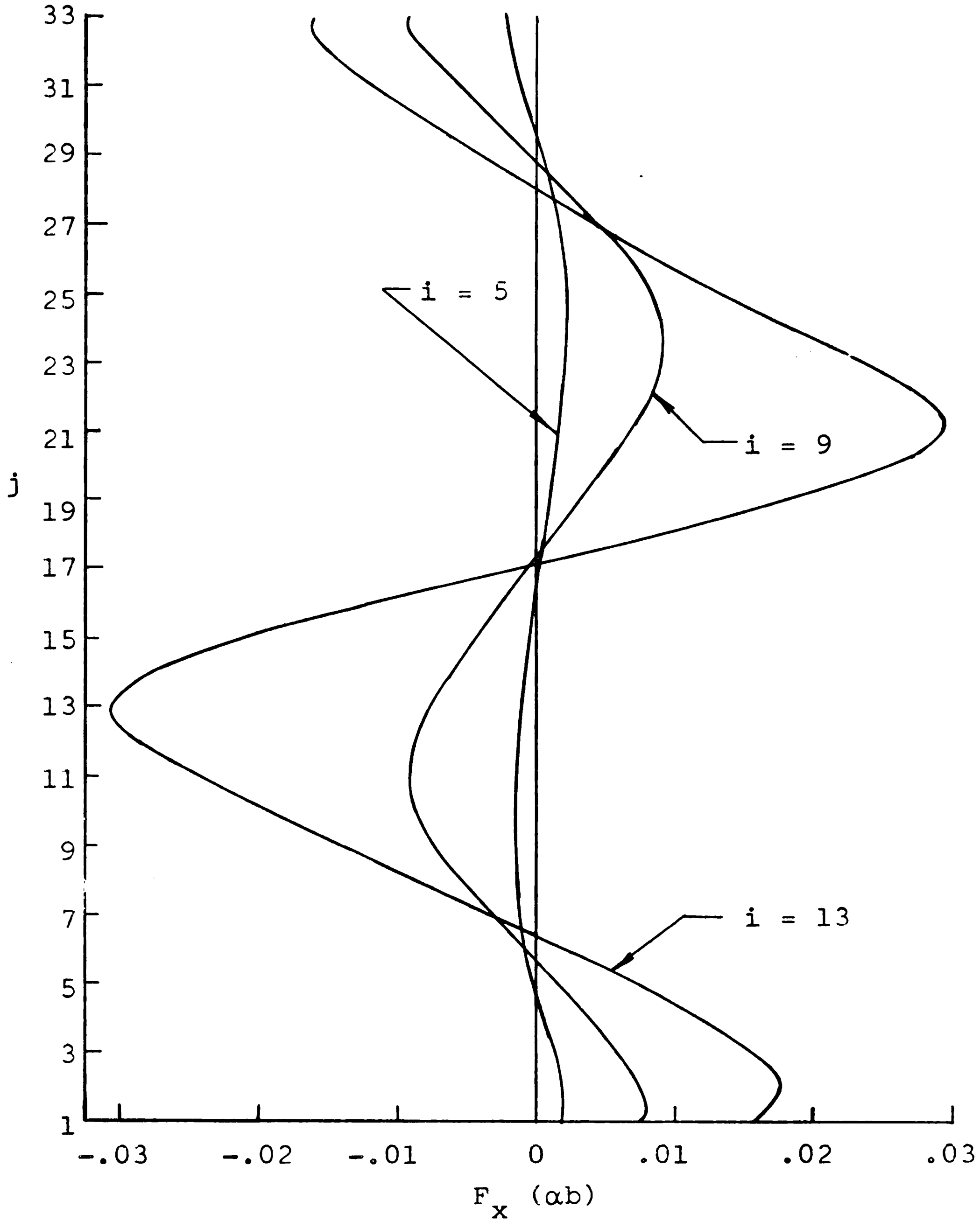


Fig. 19.--F_x versus j

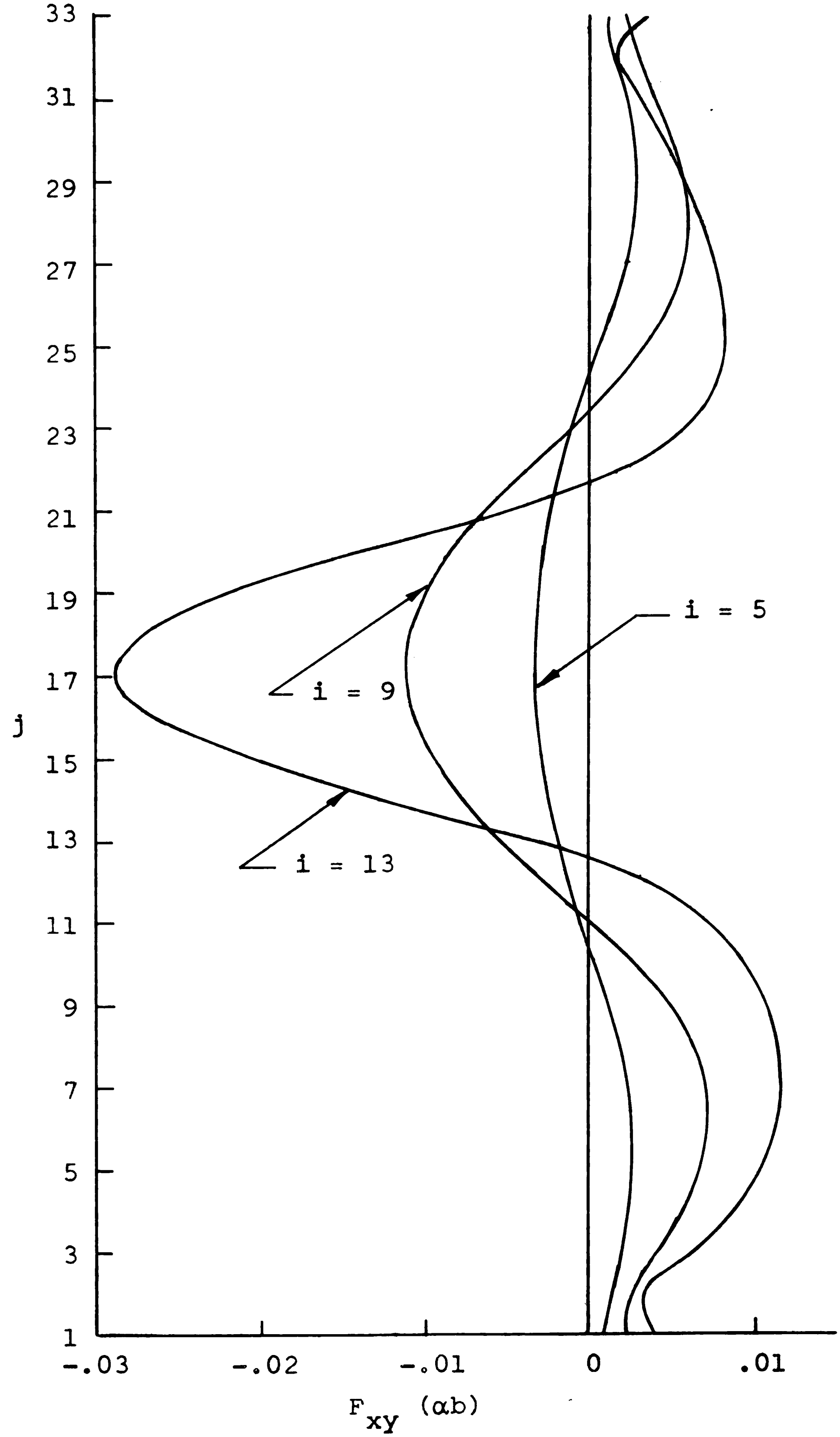


Fig. 20.--F_{xy} versus j

a qualitative examination indicates that these couples are approximately zero.

4.2. Results of the Continuum Analysis

The continuum analysis for the edge dislocation appears to give reasonable results for all system variables. The analytic portion of the solution, which solves the problem of the edge dislocation in an infinite medium, is very similar to the well-known isotropic solution given in Cottrell [2].

The superimposed numerical solution required to cancel the boundary stresses of the analytic solution comes very close to accomplishing its purpose. An examination of Tables 17, 18, and 19 shows that the boundary stresses remaining after the superposition of the two solutions have magnitudes less than 7 x 10^{-4}. The distributions of σ_x, σ_y, and τ_{xy} (shown in Figures 26, 27, and 28) are such that the net stress resultants on various sections appear to be zero. This is necessary since no external loads are applied.

Like the isotropic case discussed in Cottrell the solution contains a singularity at the origin. The u displacements on the line $x_1 = 0$ are .5b for $y_1 < 0$ and zero for $y_1 > 0$. At the origin itself u has the value $(\infty - \infty)$. The v displacement approaches negative infinity at points approaching the origin. However, large negative values of v occur only at points very near the origin. The v displacement at the point (0,.0625L) in the xy plane has the relatively small value of -.1395b.

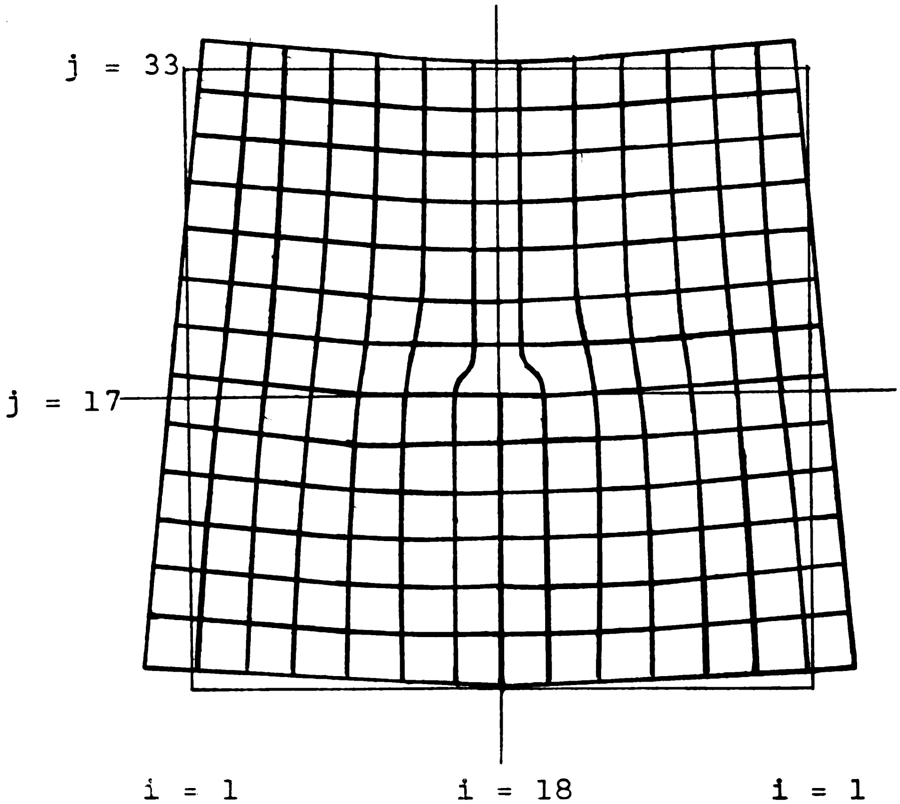


Fig. 21.--Diagrammatic representation of the distorted discrete model

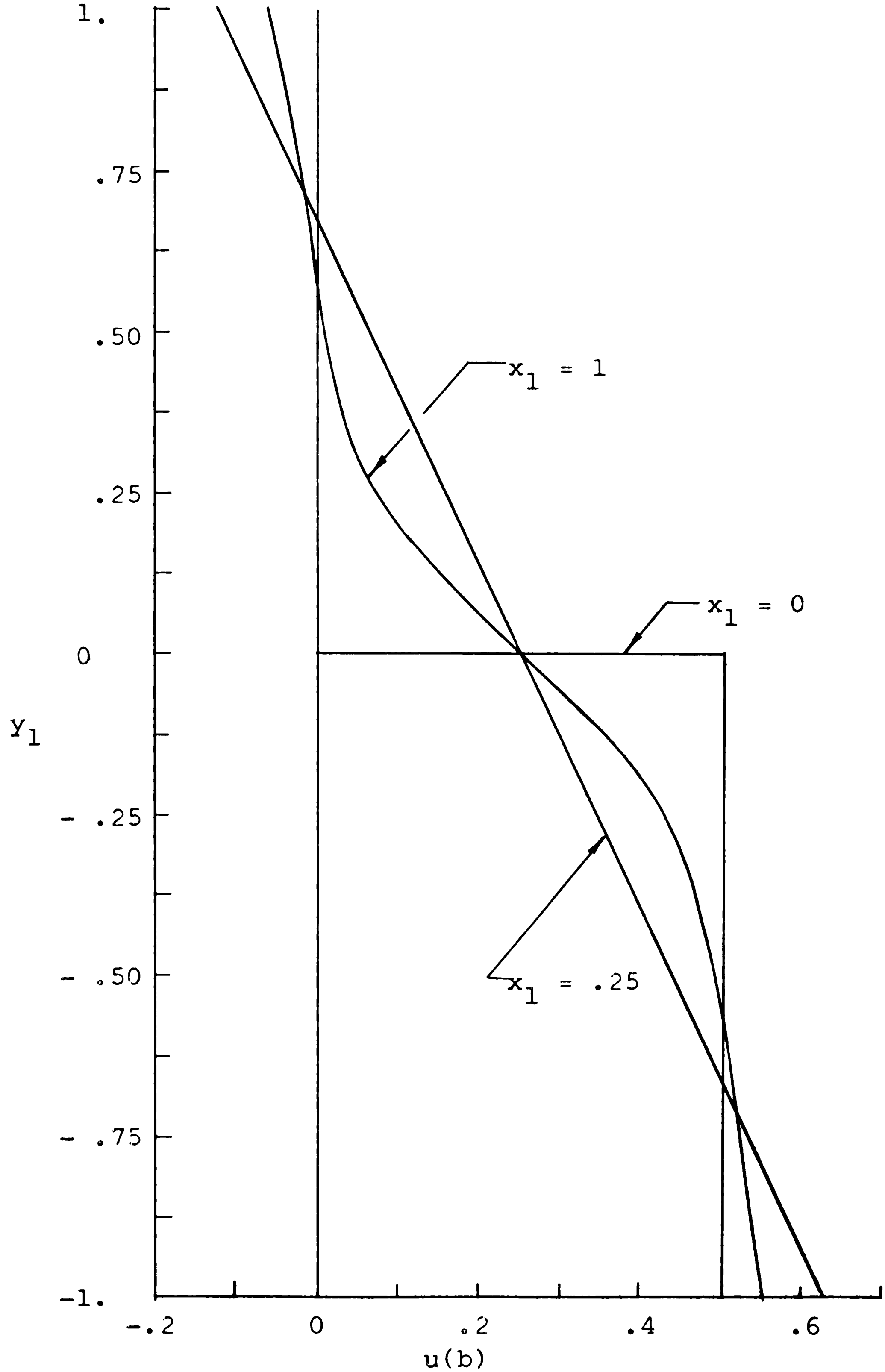


Fig. 22.--u displacement for combined continuum versus y_1

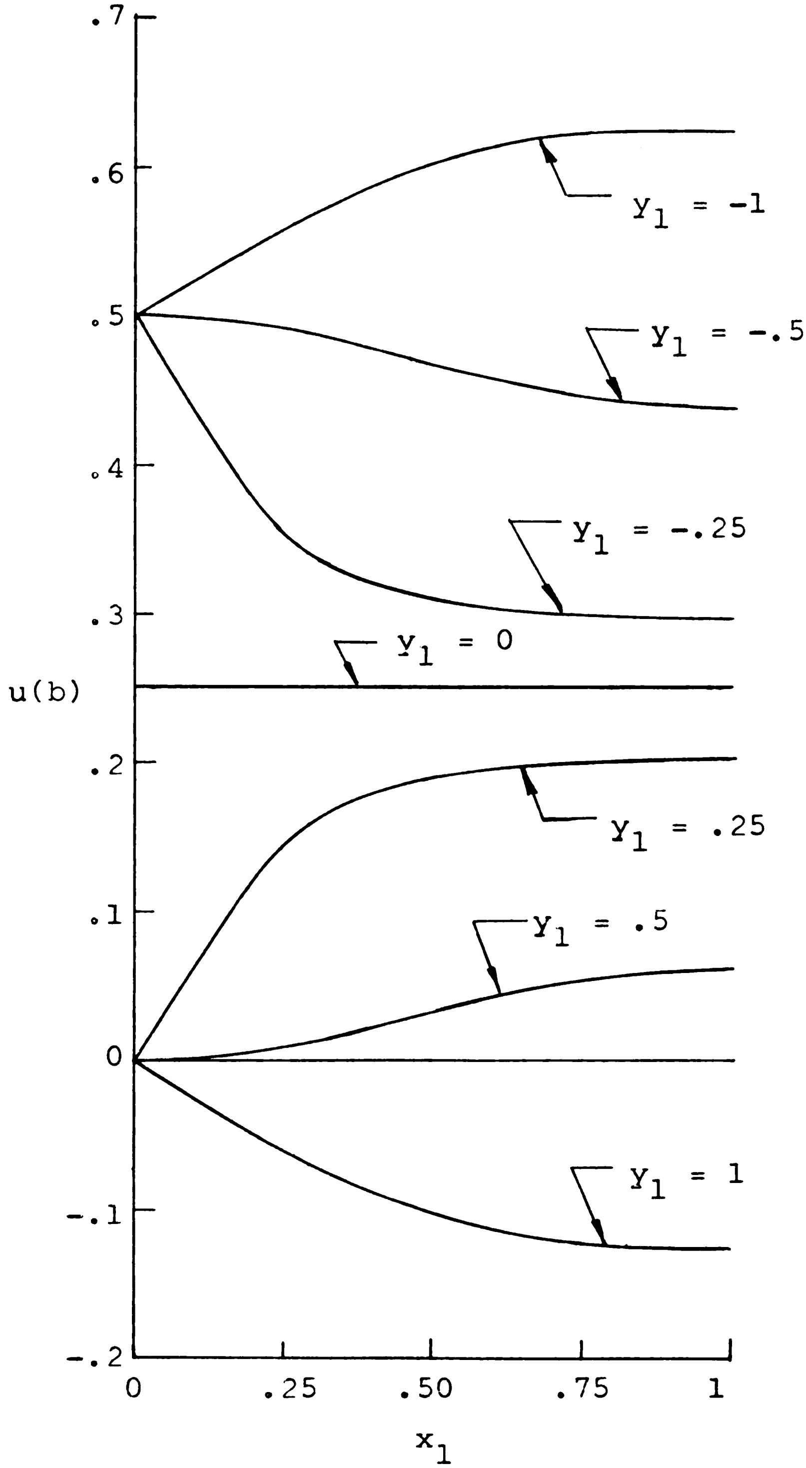


Fig. 23.--u displacement for combined continuum versus x_1

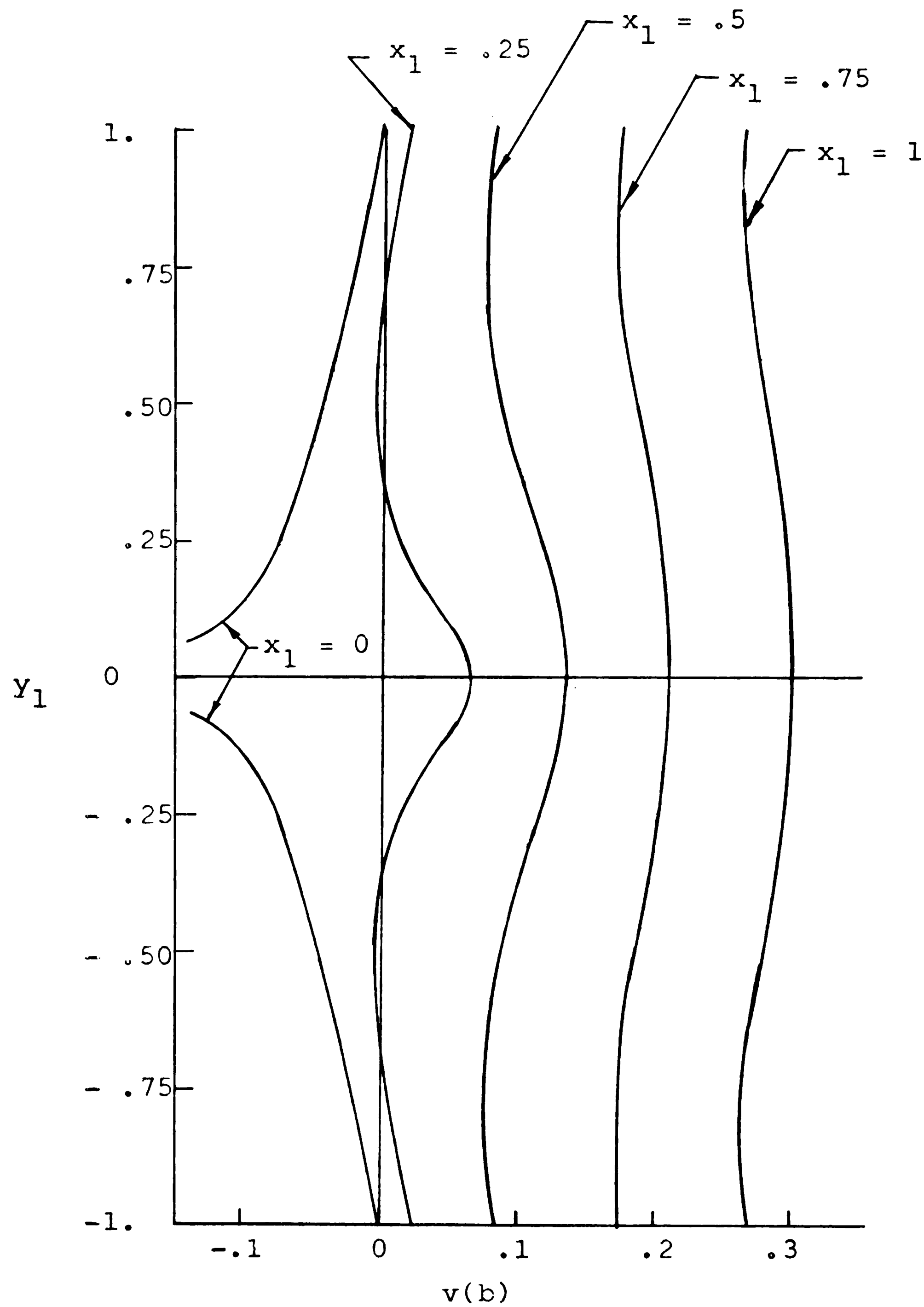


Fig. 24.--v displacement for combined continuum versus y_1

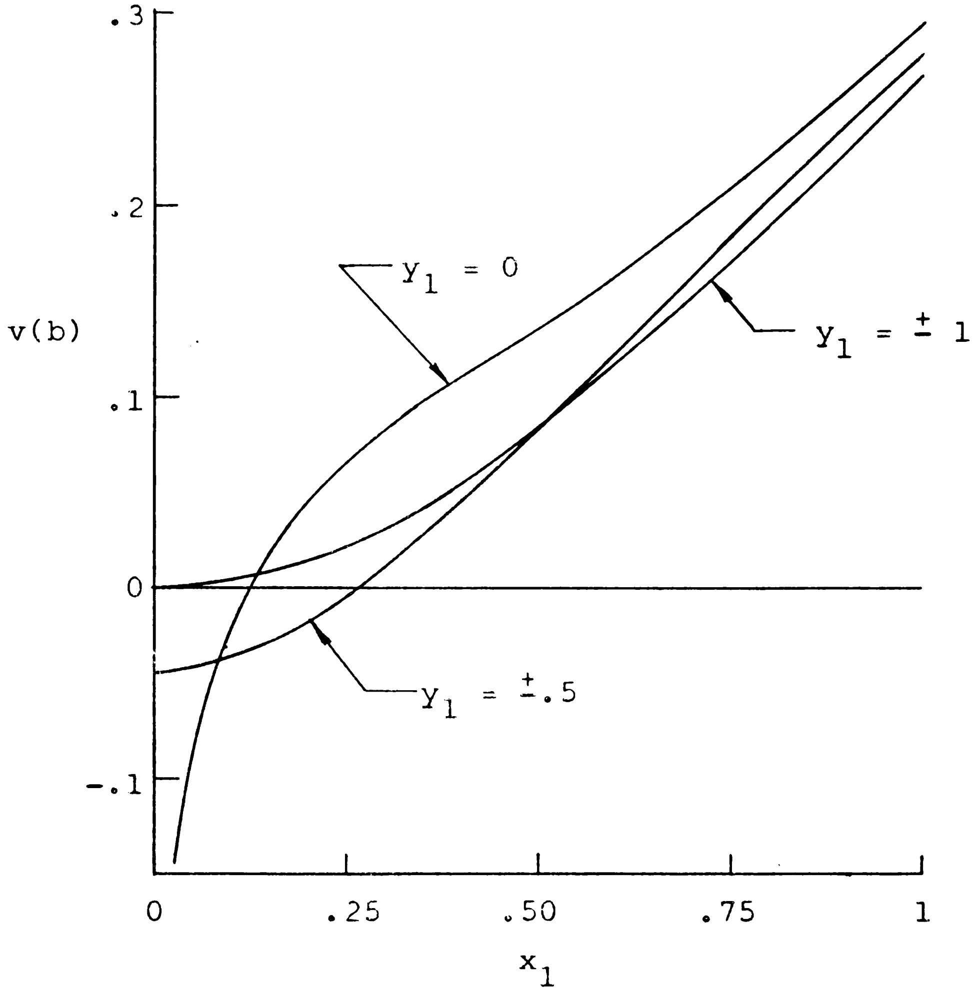


Fig. 25.--v displacement for combined continuum versus x_1

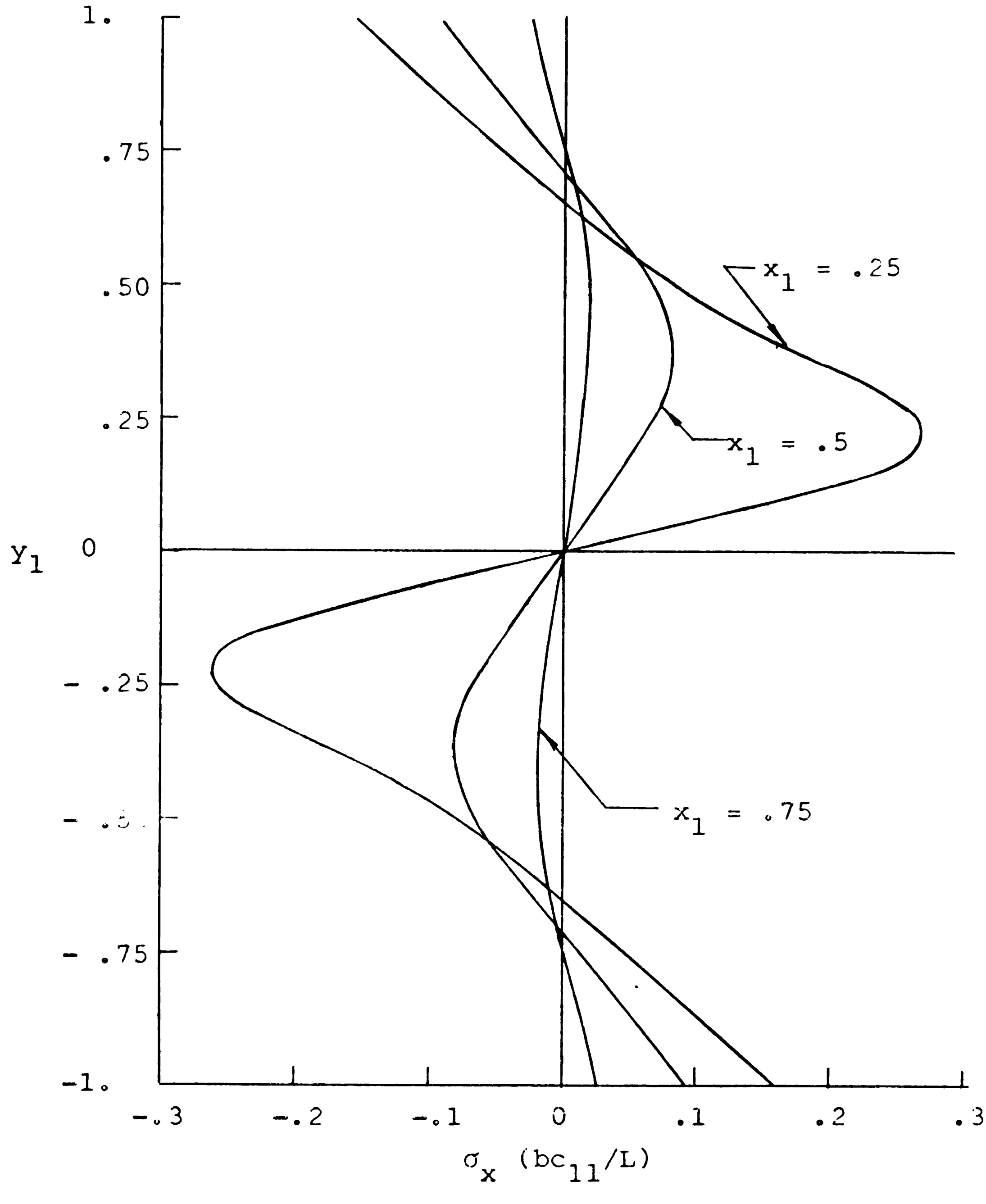


Fig. 26.--σ_x for combined continuum versus y_1

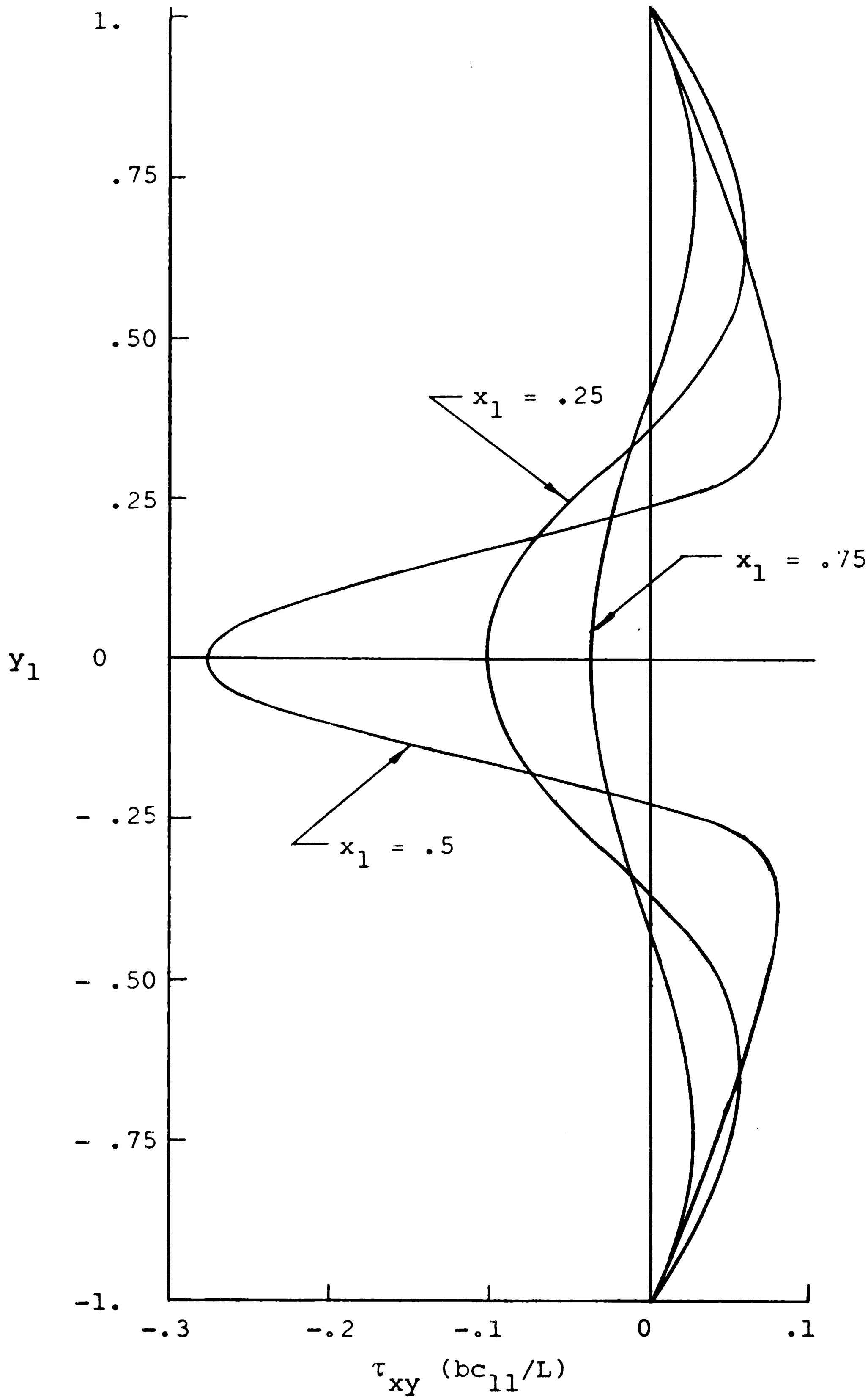


Fig. 27.--τ_{xy} for combined continuum versus y_1

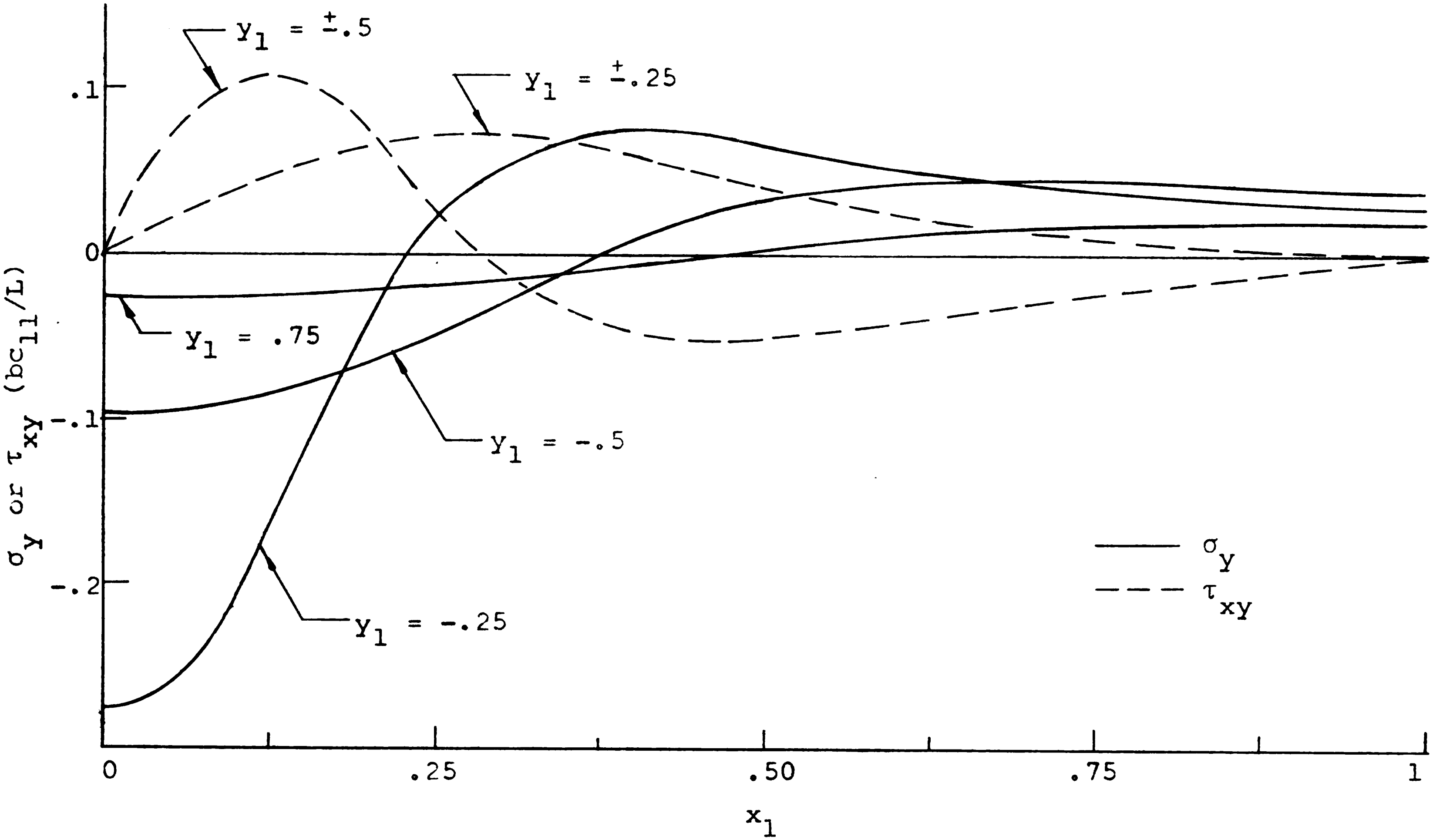


Fig. 28.—σ_y and τ_{xy} for combined continuum versus x_1

The values of stresses σ_x, σ_y, and τ_{xy} all approach either plus or minus infinity as the origin is approached. However, these stresses also have relatively small values at points near the origin. At the point (.0625L,0) τ_{xy} has the value $-1.20790bc_{11}/L$ and at the points (0, $\pm$ .0625L) σ_x and σ_y have values of $\pm 1.20790bc_{11}/L$.

For purposes of comparison of the continuum and discrete models the length .0625L in the xy continuum corresponds to the one lattice spacing, b, in the discrete material model. Therefore, the above mentioned points are located just one atomic spacing from the origin. Making the substitution

$$b = .0625L$$

into the values of stress given above results in values of stress in terms at c_{11} of $1.20790(.0625L)c_{11}/L = .07549c_{11}$. This value is large compared with macroscopic values of the elastic limit which are in the neighborhood of $c_{11}/10^3$; however, it may not be large with respect to atomic scale elastic limits. The values of stresses drop very quickly and a glance at Tables 17 through 19 shows that at points on the rectangle x = .25L, y = $\pm$.25L the stresses are all below $.2756bc_{11}/L = .01723c_{11}$.

It should be recognized that the equations of the theory of elasticity are derived on the assumption that strains are small. This assumption is necessary for geometric linearization of the equations. It is possible that the size of the displacement discontinuity relative to the dimensions of the continuous body (The discontinuity is one-thirtysecond of the length of the square body.) is such that geometric small strain is exceeded.

4.3. Comparison of Discrete and Continuum Analyses

In general a remarkable similarity exists between the results of the continuum and discrete dislocation models. Comparing the graphs of the discrete values of u_d in Figures 15 and 16 with the corresponding representation of u_c in Figures 22 and 23, it is apparent that the respective variations of u are practically identical. Table 20 shows corresponding values of u_c and u_d in adjacent columns. An examination of this table shows that while the respective variations of u are similar the magnitude of u_d is in general 10% to 20% greater than u_c.

This is due, at least in part, to the fact that the repulsive bond forces between next nearest neighbors on the extra atom plane, $i = 18$, and the neighboring plane, $i = 17$, are greater than they should be because of the linearization approximation described in Section 2.4. These larger forces tend to increase the u displacements whereas the v displacements, because of an approximate cancellation of vertical forces, should be relatively unaffected by this error. However, the similarity between corresponding values of v for the two solutions is by no means as striking as that shown by the u displacements. A comparison of Figure 17 with Figure 24 shows that a great disparity in results exists, especially in region near the extra atom plane, $i = 18$. However, in

TABLE 20

DISCRETE AND CONTINUUM VALUES OF u DISPLACEMENT AT CORRESPONDING POINTS IN UNITS OF b

y_1	j	u_c	u_d	u_c	u_d	u_c	u_d	u_c	u_d
		$x_1=.125$	$i=15$	$x_1=.25$	$i=13$	$x_1=.5$	$i=9$	$x_1=1$	$i=1$
1.	33	-.0308	-.0375	-.0593	-.0647	-.1022	-.1042	-.1236	-.1237
.75	29	-.0125	-.0138	-.0231	-.0222	-.0338	-.0285	-.0302	-.0229
.50	25	.0019	.0066	.0084	.0177	.0345	.0492	.0632	.0765
.25	21	.0264	.0475	.0706	.0988	.1308	.1528	.1572	.1740
0	17	.2500	.2869	.2500	.2804	.2500	.2739	.2500	.2700
- .25	13	.4736	.5180	.4295	.4616	.3692	.3969	.3428	.3697
- .50	9	.4981	.5646	.4916	.5454	.4655	.5064	.4368	.4780
- .75	5	.5125	.5842	.5231	.5902	.5308	.5982	.5362	.5936
-1.	1	.5308	.6285	.5593	.6584	.6022	.6962	.6236	.7127

the region of the discrete model which lies between the vertical plane i = 13 and the side boundary, i = 1, the vertical variations of v are very similar. The variation of v along horizontal planes, j = constant, in this region are also nearly identical. Figures 18 and 25 show these variations graphically and indicate an approximately constant change in v as the side boundary is approached. This constant change is nearly the same for both models.

The major difference then between the values of v for the two models in the region between i = 13 (x_1 = .25) and i = 1 (x_1 = 1) is that v_d is greater than v_c by an amount which varies from .16b to .21b. Since the discrepancy between respective values of v originates in the region adjacent to the extra atom plane, it is probable that these differences are primarily due to the fact that the dislocations were introduced into the two material models by slightly different methods.

In the method used to form the continuum dislocation, the displacement discontinuity, b, across the cut on the negative y axis is caused by normal stresses acting across this cut. The faces of the cut are assumed to be free from shear stress. In the discrete dislocation tangential forces are transmitted between the extra atom plane, i = 18, and its adjacent plane. This difference may well be the cause of the discrepancy in corresponding values of v for the two models.

It is possible to construct a continuum edge dislocation by a method which corresponds more closely to that described in Section 2.2 for the formation of the discrete dislocation. This procedure first requires the cutting of a notch of width b and height h in the continuum. Then a strip of material of width 2b and height h is elastically compressed to a width b and inserted into the notch and allowed to expand. It is necessary to make some reasonable assumption regarding the Poisson effect on the height, h, of the strip during the compression of its width, and also to choose a reasonable condition of tangential continuity across the notch-strip interface. It is obvious that the solution of such a model is much more difficult in a mathematical sense than the model analyzed in Chapter III.

Figures 26 and 27 show the distributions of σ_x and τ_{xy} on various vertical sections of the continuum model. Their discrete analogs, F_x and F_{xy}, are shown in Figures 19 and 20. Qualitatively, the distributions of corresponding values from the two solutions are almost exactly identical. In order to compare the magnitudes of discrete and continuum quantities at corresponding points, it is necessary to convert the respective values to similar units. Suppose that at a particular point σ_x has magnitude A and its discrete counterpart F_x has a value B. All stresses are written in terms of the factor bc_{11}/L while discrete quantities include the factor αb. These factors include the dimensions of the respective quantities

$$\sigma_x = A \frac{bc_{11}}{L} \tag{4.1}$$

$$F_x = B\alpha b. \tag{4.2}$$

If F_x is assumed to be uniformly distributed over an area one lattice spacing square, a quantity which is dimensionally similar to stress is the result

$$\frac{F_x}{b^2} = B\,\frac{\alpha}{b}. \tag{4.3}$$

Geometric similarity of the two models requires that

$$b = L/16 \tag{4.4}$$

and in Appendix IV it is shown that elastic similarity requires that

$$\alpha = \frac{bc_{11}}{2}. \tag{4.5}$$

Substituting (4.4) and (4.5) into (4.3) gives

$$\frac{F_x}{b^2} = B\,\frac{\frac{bc_{11}}{2}}{\frac{L}{16}} = 8B\,\frac{bc_{11}}{L}\,. \tag{4.6}$$

Therefore in order to compare the magnitudes of F_x and F_{xy} with σ_x and τ_{xy}, the latter should be multiplied by the factor eight. Table 21 gives values of discrete and continuum stress at corresponding geometric positions in adjacent columns. An examination of this table shows that the magnitudes of corresponding quantities are quite similar.

In summary it may be said that the u displacements for the two solutions are very nearly the same. If the linearization error of the discrete solution could be corrected, the discrete values of u would be reduced and similarity would most probably be improved. It is notable that the similarity between u_c and u_d extends almost to the extra atom plane. A comparison of u_c values on x_1 =

TABLE 21

CONTINUUM AND DISCRETE STRESSES AT

CORRESPONDING POINTS (bc_{11}/L)

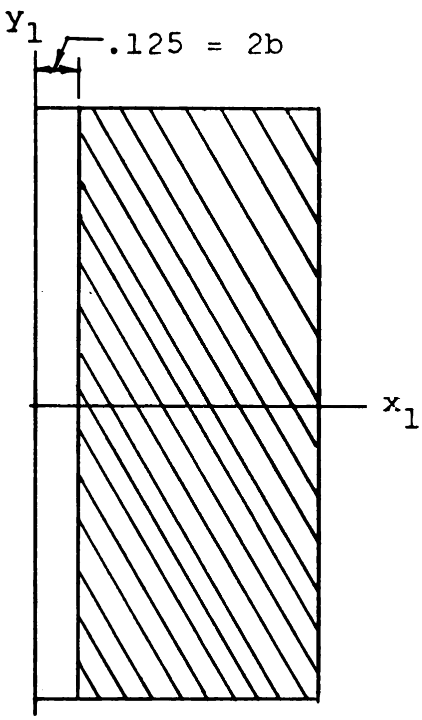
		σ_x	$\frac{F_x}{b^2}$	τ_{xy}	$\frac{F_{xy}}{b^2}$
y_1	j	x=.25	i=13	x=.25	i=13
1.	33	-.1588	-.1231	.0004	.0275
.75	29	-.0450	-.0176	.0406	.0445
.50	25	.0811	.1023	.0712	.0649
.25	21	.2575	.2345	.0261	-.0411
0	17	0	-.0106	-.2756	-.2310
- .25	13	-.2575	-.2446	.0261	-.0308
- .50	9	-.0811	-.1119	.0712	.0858
- .75	5	.0450	.0558	.0406	.0835
-1.	1	.1588	.1271	.0004	.0395
		σ_x	$\frac{F_x}{b^2}$	τ_{xy}	$\frac{F_{xy}}{b^2}$
y_1	j	x_1=.5	i=9	x_1=.5	i=9
1.	33	-.0927	-.0679	.0007	.0182
.75	29	-.0126	-.0384	.0493	.0452
.50	25	.0647	.0644	.0409	.0253
.25	21	.0682	.0545	-.0489	-.0518
0	17	0	.0044	-.1034	-.0891
- .25	13	-.0682	-.0610	-.0489	-.0436
- .50	9	-.0647	-.0593	.0409	.0387
- .75	5	.0126	.0127	.0493	.0529
-1.	1	.0927	.0612	.0007	.0172

.125 with u_d values on i = 15 (see Table 20) shows that differences between u_c and u_d on a vertical plane only two lattice spacings from the extra atom plane are no larger than for points on the side boundary.

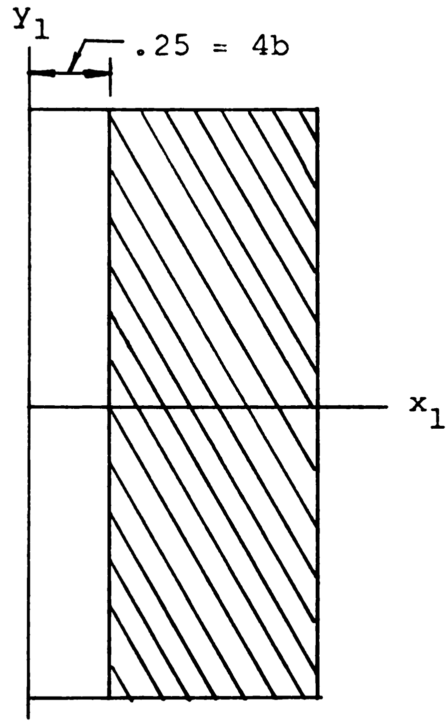
Respective values of v for the two solutions show a much greater disparity than the u values. This disparity is believed to result from the fact that no shear stress acts on the sides of the cut in the continuum dislocation while in the discrete dislocation shearing forces are transmitted between the extra atom plane and its neighboring plane. In the region $.25 \leq x_1 \leq 1$ of the continuum model which corresponds approximately with the discrete region where $13 \geq i \geq 1$, the relative v displacements for the two solutions show great similarity.

This situation is certainly a manifestation of the principle of Saint Venant which states that the effects of different but statically equivalent boundary stresses are virtually identical except at points near the boundary.

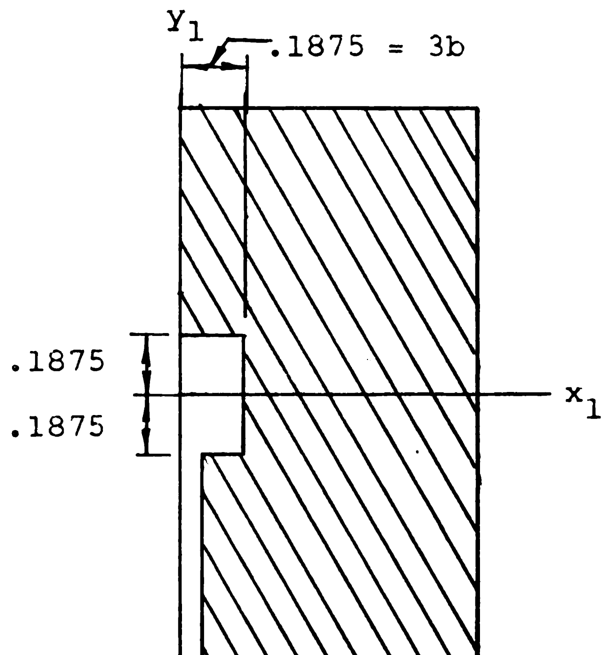
Figure 29 pictorially illustrates three regions of similarity common to the two dislocation models. Figure 29a indicates with cross-hatching the region in which the u displacements, both relative and absolute, for the two models show a particular similarity. This region excludes only the strip of material lying within a distance 2b = .125L of the vertical axis of symmetry. Figure 29b shows the region in which the relative values of v_c and v_d closely resemble one another. Figure 29c



(a) Region in which u_c and u_d are similar



(b) Region in which relative values of v_c and v_d are similar



(c) Region in which relative displacements of both the continuum and discrete solution are less than .05

Fig. 29.--Regions of similarity for the continuum and discrete models (cross-hatched)

shows the region in which both the relative displacements for the discrete solution and the strains for the continuum solution are all less than .05 or 5%. The approximate values of the continuum strains were determined by scaling slopes from Figures 22 through 25. The significance of the value 5% is that for a relative displacement of 5% or less from the equilibrium atomic spacing a linear force displacement relationship is approximately correct. Johnston and Gilman, in tests of single crystals of lithium flouride reported linear elastic strains of up to 5% [13]. Neither of the two models can be expected to accurately represent the configuration of a real edge dislocation in the non-crosshatched region of Figure 29c, simply because the linear force (stress) relative displacement (strain) approximation is not true for relative displacements (strains) of the size encountered in this region. It is certainly apparent, however, that the discrete solution, even though it predicts linear relative displacements of nearly 60% for certain lattice pairs, is much closer to reality than a continuum solution which predicts infinite displacements, strains, and stresses at a particular point.

Stresses and lattice forces on several corresponding vertical sections are practically identical both with regard to distribution and magnitude. The comparisons between stress and lattice force were all made on vertical sections which lie in the cross-hatched portion of Figure 29b. In this region relative values of u and v for both solutions are very similar and they are also small (under 5%). Since stresses and lattice forces depend directly on relative displacements, and since the accuracy of these quantities requires that the relative displacements be small, good similarity between lattice forces and stresses is assured in this region.

The most surprising result of the comparison of the discrete and continuum solutions is the great similarity of all system variables at points which are very close to the center of the dislocation at $x_1 = 0$, $y_1 = 0$. Cottrell has estimated that the region to which the elastic dislocation solution applies lies outside a cylinder of radius 10b centered on the point (0,0) [2]. Comparison of the discrete and a continuum solutions here indicates that they show great similarity at points which lie only 4b from the dislocation center. If the discrete solution is accepted as giving a reasonable description of an edge dislocation, this indicates that the elastic dislocation solution may be accurately applied at points far closer to the dislocation center than the previously accepted limiting distance of 10b.

V. POSSIBLE EXTENSIONS OF RESEARCH

In Section 4.3 two causes for differences in the results of the two solutions were mentioned. The most obvious extension of the work of this dissertation is to eliminate these two causes.

A technique to construct a continuum dislocation in a way which approximates the method used in Chapter II to produce the discrete dislocation was described in Section 4.3. An actual theory of elasticity analysis of this problem is difficult, perhaps too difficult to justify an attempted solution since it is questionable whether the tangential effects between the strip and the notch may be made similar to the analogous discrete effect. Similarity in the construction of the two dislocations may also be achieved by creating a discrete dislocation by the method described in Section 3.1 for the creation of a continuum dislocation. This involves the insertion of a rigid strip of material of width 2b and height sb (see Figure 5) into the gap between $i = r$ and $i = r + 1$. It is then assumed that no tangential forces are transmitted between the rigid block and the lattice points on $i = r$ and $i = r + 1$.

Equilibrium equations may then be written for each lattice point with $u_{i,j}$ and $v_{i,j}$ as unknowns at all points except those in contact with the rigid block. Here the u displacement is a known value, .5b for the symmetrical case, and the normal force between the block and the lattice point is unknown. The vertical displacement is the other unknown associated with such points. If the discrete dislocation is formed in this way, both of the conditions mentioned in Section 4.3 as contributing to the differences in the solutions would be corrected.

If the method described in Section 2.2 for the formation of the discrete edge dislocation is retained (The author believes that this is physically a more realistic method.), then an attempt may be made to improve the poor approximation involved in linearizing the forces between next nearest neighbors on the extra atom plane and the adjacent plane. As a first improvement these forces may be left in the non-linearized form. Forces in the rest of the lattice may still be expressed in linearized form since relative displacements there are small enough so that the linearizing approximation is not seriously inaccurate. Solution of this mixed system of linear and non-linear equations may then be attempted by an iteration technique. If convergence occurs, some improvement in results is expected. If the iteration does not converge, the attempt would have to be abandoned.

Another possible improvement might be to assume a simple Lennard-Jones force potential between lattice pairs on the extra atom plane and the adjacent plane while retaining a linear force (linearized in terms of u and v) elsewhere. Here again, a solution must be attempted before there is any assurance that it can be found.

In Kittel it is pointed out that the central force condition

$$c_{12} = c_{44}$$

is not true for most of the common metals such as copper, aluminum, or iron [10]. A discrete model more nearly approximating a metal must take into account forces which are transverse to the line joining the individual lattice points.

More complex edge dislocation problems might be attempted either with the model used in this dissertation or with an improved model. These problems may include a non-symmetrical case of the problem solved here or a lattice containing more than one dislocation. The limiting factor in attempting a solution of more involved dislocation problems is that a reasonably large crystal lattice is necessary in order that the solution have any physical significance. The large lattice, of course, involves a large number of unknowns, and the solution of such large systems, even if possible, requires a prohibitively large amount of computer time. The convergence of the iteration for the problem considered here, which involved 1139 unknowns, took 30 minutes of computer time.

It may be possible to use a composite material model to describe the more complex dislocation problems.

Since the results of the continuum and discrete analyses are very close except in the region near the dislocation, a model consisting of a continuous region with discrete lattices in the vicinity of dislocations may be a possibility.

Departing completely from the consideration of dislocations in crystal lattices, the similarity of results for the discrete and continuum models indicates that it may be advantageous to directly simulate the elastic continuum by a ball and spring system. This technique has been used for analyses, usually dynamic, of such complex composite structures as building frames and airplane wings but has found little use in continuous bodies. If this simulation could be done more or less by inspection, an advantage would be gained over the accepted practice of formulating the problem with the partial differential equations of elasticity and then approximating them by difference equations. This technique has been used in the solution of problems involving torsion of prismatic bars. A membrane analogy is used initially and then the stretched membrane is directly simulated by a net of nodal points connected by stretched strings with pressure loads concentrated at the nodal points.

This direct simulation may be especially advantageous for materials with complex stress-strain relationships. It may also be possible to simulate visco-elastic materials by nodal points connected by means of spring-dashpot combinations.

APPENDIX I

EQUILIBRIUM EQUATIONS FOR THE DISCRETE MODEL IN A PARTICULAR EXAMPLE

A. For the case $\alpha = B$

$m = 34$

$n = 33$

$r = 17$

$s = 17$

(Parameters m, n, r, s are defined in Figure 5 .) The equilibrium equations (2.10) through (2.13) and (2.24) through (2.49) have the form

$2 \leq i \leq 16$

$2 \leq j \leq 32.$

$$\sum F_x = 0 \qquad -4u_{i,j} + u_{i+1,j} + u_{i-1,j} + .5(u_{i+1,j+1} + v_{i+1,j+1} + u_{i+1,j-1} - v_{i+1,j-1} + u_{i-1,j+1} - v_{i-1,j+1} + u_{i-1,j-1} + v_{i-1,j-1}) = 0.$$

$$\sum F_y = 0 \qquad -4v_{i,j} + v_{i,j+1} + v_{i,j-1} + .5(u_{i+1,j+1} + v_{i+1,j+1} - u_{i+1,j-1} + v_{i+1,j-1} - u_{i-1,j+1} + v_{i-1,j+1} + u_{i-1,j-1} + v_{i-1,j-1}) = 0.$$

$i = 1$

$j = 1$

$\sum F_x = 0 \qquad -1.5u_{1,1} + u_{2,1} + .5(u_{2,2} + v_{2,2} - v_{1,1}) = 0.$

$\sum F_y = 0 \qquad -1.5v_{1,1} + v_{1,2} + .5(u_{2,2} + v_{2,2} - u_{1,1}) = 0.$

$i = 1$

$2 \leq j \leq 32$

$\sum F_x = 0 \qquad -2u_{1,j} + u_{2,j} + .5(u_{2,j+1} + v_{2,j+1} + u_{2,j-1} -$

$v_{2,j-1}) = 0.$

$\sum F_y = 0 \qquad -3v_{1,j} + v_{1,j+1} + v_{1,j-1} + .5(u_{2,j+1} + v_{2,j+1} -$

$u_{2,j-1} + v_{2,j-1}) = 0.$

$i = 1$

$j = 33$

$\sum F_x = 0 \qquad -1.5u_{1,33} + u_{2,33} + .5(u_{2,32} - v_{2,32} +$

$v_{1,33}) = 0.$

$\sum F_y = 0 \qquad -1.5v_{1,33} + v_{1,32} + .5(v_{2,32} - u_{2,32} +$

$u_{1,33}) = 0.$

$2 \leq i \leq 16$

$j = 33$

$\sum F_x = 0 \qquad -3u_{i,33} + u_{i+1,33} + u_{i-1,33} + .5(u_{i+1,32} -$

$v_{i+1,32} + u_{i-1,32} + v_{i-1,32}) = 0$

$\sum F_y = 0 \qquad -2v_{i,33} + v_{i,32} + .5(v_{i+1,32} - u_{i+1,32} +$

$v_{i-1,32} + u_{i-1,32}) = 0.$

$i = 17$

$j = 33$

$\sum F_x = 0 \quad -4u_{17,33} + u_{16,33} + .5(-u_{17,32} - v_{17,32} + u_{16,32} + v_{16,32}) = 0$

$\sum F_y = 0 \quad -2v_{17,33} + v_{17,32} + .5(v_{17,32} + u_{17,32} + v_{16,32} + u_{16,32}) = 0.$

$i = 17$

$19 \leq j \leq 32$

$\sum F_x = 0 \quad -5u_{17,j} + u_{16,j} + .5(-u_{17,j+1} + v_{17,j+1} + u_{16,j+1} - v_{16,j+1} + u_{16,j-1} + v_{16,j-1} - u_{17,j-1} - v_{17,j-1}) = 0$

$\sum F_y = 0 \quad -4v_{17,j} + 1.5(v_{17,j+1} + v_{17,j-1}) + .5(-u_{17,j+1} + v_{16,j+1} - u_{16,j+1} + v_{16,j-1} + u_{16,j-1} + u_{17,j-1}) = 0.$

$i = 17$

$j = 18$

$\sum F_x = 0 \quad -5.2u_{17,18} + u_{16,18} + .5(u_{16,19} - v_{16,19} - u_{17,19} + v_{17,19} + u_{16,17} + v_{16,17} - u_{17,17}) + .4(v_{17,18} - v_{18,17}) = .13246b$

$\sum F_y = 0 \quad -4.8v_{17,18} + 1.5(v_{17,19} + v_{17,17}) + .5(-u_{16,19} + v_{16,19} - u_{17,19} + u_{16,17} + v_{16,17} + u_{17,17}) + .4u_{17,18} + .8v_{18,17} = -.26492b.$

$i = 17$

$j = 17$

$\sum F_x = 0 \qquad -3.7u_{17,17} + u_{16,17} + .5(-u_{17,18} + v_{17,18} + u_{16,18} - v_{16,18} + u_{16,16} + v_{16,16}) - .1v_{17,17} - .4v_{18,16} = .63246b$

$\sum F_y = 0 \qquad -4.3v_{17,17} + v_{17,18} + v_{17,16} + .5(-u_{17,18} + v_{17,18} - u_{16,18} + v_{16,18} + v_{16,16} + u_{16,16}) - .1u_{17,17} + .8v_{18,16} = -.26492b.$

$i = 17$

$2 \leq j \leq 16$

$\sum F_x = 0 \qquad -3.4u_{17,j} + u_{18,j} + u_{16,j} + .5(u_{16,j+1} - v_{16,j+1} + u_{16,j-1} + v_{16,j-1}) + .4(v_{18,j+1} - v_{18,j-1}) = .76492b$

$\sum F_y = 0 \qquad -4.6v_{17,j} + v_{17,j+1} + v_{17,j-1} + .5(-u_{16,j+1} + v_{16,j+1} + u_{16,j-1} + v_{16,j-1}) + .8(v_{18,j+1} + v_{18,j-1}) = 0.$

$i = 17$

$j = 1$

$\sum F_x = 0 \qquad -2.7u_{17,1} + u_{16,1} + .5(u_{16,2} - v_{16,2}) + .4v_{18,2} + .1v_{17,1} = .63246b$

$\sum F_y = 0 \quad -2.3v_{17,1} + v_{17,2} + .5(-u_{16,2} + v_{16,2}) +$

$.1u_{17,1} + .8v_{18,2} = .26492b.$

$i = 18$

$j = 1$

$\sum F_y = 0 \quad -2.6v_{18,1} + v_{18,2} + 1.6v_{17,2} - .8u_{17,2} = .52982b.$

$i = 18$

$2 \leq j \leq 16$

$\sum F_y = 0 \quad -5.2v_{18,j} + v_{18,j+1} + v_{18,j-1} + 1.6(v_{17,j-1} +$

$v_{17,j+1}) + .8(u_{17,j-1} - u_{17,j+1}) = 0.$

$i = 18$

$j = 17$

$\sum F_y = 0 \quad -4.2v_{18,17} + v_{18,16} + .8(u_{17,16} - u_{17,18}) +$

$1.6(v_{17,16} + v_{17,18}) = 0.$

$2 \leq i \leq 16$

$j = 1$

$\sum F_x = 0 \quad -3u_{i,1} + u_{i+1,1} + u_{i-1,1} + .5(u_{i+1,2} +$

$v_{i+1,2} + u_{i-1,2} - v_{i-1,2}) = 0$

$\sum F_y = 0 \quad -2v_{i,1} + v_{i,2} + .5(u_{i+1,2} + v_{i+1,2} -$

$u_{i-1,2} + v_{i-1,2}) = 0.$

B. The solution of the system of equations in Section A indicates that the assumption that next nearest neighbor bonds between lattice points on the columns i = 17 and i = 18 do not rotate appreciably from their original 2 to 1 slope should be changed. This change consists of a new assumption that all these bonds have a slope of 1 to 1 except that bond between the lattice points (17,18) and (18,17) which retains its original 2 to 1 slope and the bond between (17,17) and (18,16) which is assumed to be 1 to 0.8. On the basis of the solution of the system of Section A these slopes are believed to be more realistic. The equilibrium equations which are affected by these changes are shown below in their corrected form.

For $i = 17$

$j = 17$

$\sum F_x = 0$ $\quad -3.77936u_{17,17} + u_{16,17} + .5(-u_{17,18} + v_{17,18} + u_{16,16} + v_{16,16} + u_{16,18} - v_{16,18}) + .05872v_{17,17} - .55872v_{18,16} = .68507b$

$\sum F_y = 0$ $\quad -4.19841v_{17,17} + 1.5(v_{17,18} + v_{17,16}) + .5(-u_{17,18} + u_{16,16} + v_{16,16} - u_{16,18} + v_{16,18}) - .15080u_{17,17} + .69841v_{18,16} = -.23127b.$

For $i = 17$

$2 \le j \le 16$

$\sum F_x = 0$ $\quad -3.63246u_{17,j} + u_{16,j} + .5(u_{16,j+1} - v_{16,j+1} + u_{16,j-1}) - .63246(v_{18,j-1} - v_{18,j+1}) = .91886b$

$\sum F_y = 0 \quad -4.26492v_{17,j} + v_{17,j+1} + v_{17,j-1} +$

$.5(u_{16,j-1} + v_{16,j-1} - u_{16,j+1} + v_{16,j+1}) +$

$.63246(v_{18,j-1} + v_{18,j+1}) = 0.$

For $i = 17$

$j = 1$

$\sum F_x = 0 \quad 2.81623u_{17,1} + u_{16,1} + .5(u_{16,2} - v_{16,2} +$

$v_{17,1}) + .63246(v_{18,2} - v_{17,1}) = .70943b$

$\sum F_y = 0 \quad -2.13246v_{17,1} + v_{17,2} + .5(-u_{16,2} + v_{16,2}) +$

$.18377u_{17,1} + .63246v_{18,2} = .20943b.$

For $i = 18$

$2 \leq j \leq 15$

$\sum F_y = 0 \quad -4.52984v_{18,j} + v_{18,j+1} + v_{18,j-1} -$

$.63246(u_{17,j+1} - u_{17,j-1}) + 1.26492(v_{17,j+1} +$

$v_{17,j-1}) = 0.$

For $i = 18$

$j = 16$

$\sum F_y = 0 \quad -4.66174v_{18,16} + v_{18,17} + v_{18,15} +$

$.63246u_{17,15} + 1.26492v_{17,15} - .69841u_{17,17} +$

$1.39682v_{17,17} = .04170b.$

For $i = 18$

$j = 17$

$$\sum F_y = 0 \qquad -3.86492v_{18,17} + v_{18,16} + .63246u_{17,16} + 1.26492v_{17,16} - .8u_{17,18} + 1.6v_{17,18} = -.19764b.$$

APPENDIX II

DETERMINATION OF THE FORM OF DISPLACEMENTS FOR THE CASE OF PLANE STRAIN AND CUBIC SYMMETRY AND WITH A DISCONTINUOUS DISPLACEMENT

The equilibrium equations for plane strain and cubic symmetry with no body force are

$$
\begin{aligned}
c_{11}\frac{\partial^2 u}{\partial x^2} + (c_{12} + c_{44})\frac{\partial^2 v}{\partial x\,\partial y} + c_{44}\frac{\partial^2 u}{\partial y^2} &= 0 \\
c_{11}\frac{\partial^2 v}{\partial y^2} + (c_{12} + c_{44})\frac{\partial^2 u}{\partial x\,\partial y} + c_{44}\frac{\partial^2 v}{\partial x^2} &= 0.
\end{aligned}
\qquad (1)
$$

Following the example of Eshelby [5] assume a solution to equations (1) and (2) to be

$$
\begin{aligned}
u &= A_1 f(x + py) \\
v &= A_2 f(x + py)
\end{aligned}
\qquad (2)
$$

where A_1 and A_2 are constants. Assuming the solution (2) evaluate the various derivatives which appear in the equations (1) and make the appropriate substitutions. As an example the second partial of v with respect to y is found in the following way:

$$
\frac{\partial v}{\partial y} = A_2 \frac{df}{d(x + py)} \frac{\partial(x + py)}{\partial y} = A_2 p \frac{df}{d(x + py)}
$$

$$\frac{\partial^2 v}{\partial y^2} = \frac{\partial}{\partial y}[A_2 p \frac{df}{d(x + py)}] = A_2 p \frac{d^2 f}{d^2(x + py)} \frac{\partial (x + py)}{\partial y} =$$

$$A_2 p^2 \frac{d^2 f}{d^2(x + py)} = A_2 p^2 f''.$$

In a similar manner

$$\frac{\partial^2 u}{\partial x^2} = A_1 f''$$

$$\frac{\partial^2 u}{\partial y^2} = A_1 p^2 f''$$

$$\frac{\partial^2 u}{\partial x \partial y} = A_1 p f''$$

$$\frac{\partial^2 v}{\partial x^2} = A_2 f''$$

$$\frac{\partial^2 v}{\partial x \partial y} = A_2 p f''.$$

Substitution of these derivatives into the equations (1) and cancellation of the common factor f'' shows that the equations (2) are solutions of (1) if A_1, A_2, and p satisfy the equations

$$\begin{aligned} A_1(c_{11} + c_{44}p^2) + A_2(c_{12} + c_{44})p &= 0 \\ A_1(c_{12} + c_{44})p + A_2(c_{11}p^2 + c_{44}) &= 0. \end{aligned} \tag{3}$$

If A_1 and A_2 are non-zero the determinant of their coefficients must be zero.

$$\begin{vmatrix} c_{11} + c_{44}p^2 & (c_{12} + c_{44})p \\ (c_{12} + c_{44})p & (c_{11}p^2 + c_{44} \end{vmatrix} = c_{11}c_{44}p^4 + (c_{11}{}^2 + c_{44}{}^2 -$$

$$c_{12}{}^2 - 2c_{12}c_{44} - c_{44}{}^2)p^2 + c_{11}c_{44} = 0$$

$$p^4 - \frac{(2c_{12}c_{44} + c_{12}^2 - c_{11}^2)}{c_{11}c_{44}} p^2 + 1 = 0. \tag{4}$$

Solving the characteristic equation (4) for p^2 gives

$$p^2 = \frac{2c_{12}c_{44} + c_{12}^2 - c_{11}^2}{2c_{11}c_{44}} \pm [(\frac{2c_{12}c_{44} + c_{12}^2 - c_{11}^2}{2c_{11}c_{44}})^2 - 1]^{1/2}. \tag{5}$$

Let

$$\frac{2c_{12}c_{44} + c_{12}^2 - c_{11}^2}{2c_{11}c_{44}} = \zeta .$$

Then equation (5) becomes

$$p^2 = \zeta \pm (\zeta^2 - 1)^{1/2}. \tag{6}$$

For the case of real cubic crystals Eshelby [5] points out that $\zeta^2 < 1$ (for the example in Chapter III $\zeta^2 = 1/16$), in which case p^2 is a complex number

$$p^2 = \zeta + i(1 - \zeta^2)^{1/2} \tag{7}$$

$$p^2 = \zeta - i(1 - \zeta^2)^{1/2}. \tag{8}$$

Referring to Figure 30a the equation (7) may be written in polar form

$$p^2 = \cos(2\eta + 2n\pi) + i \sin(2\eta + 2n\pi). \tag{9}$$

The angle η is defined by the following equations:

$$\cos 2\eta = \zeta$$

$$\eta = \frac{1}{2}\cos^{-1}\zeta = \frac{1}{2}\cos^{-1}\frac{2c_{12}c_{44} + c_{12}^2 - c_{11}^2}{2c_{11}c_{44}}.$$

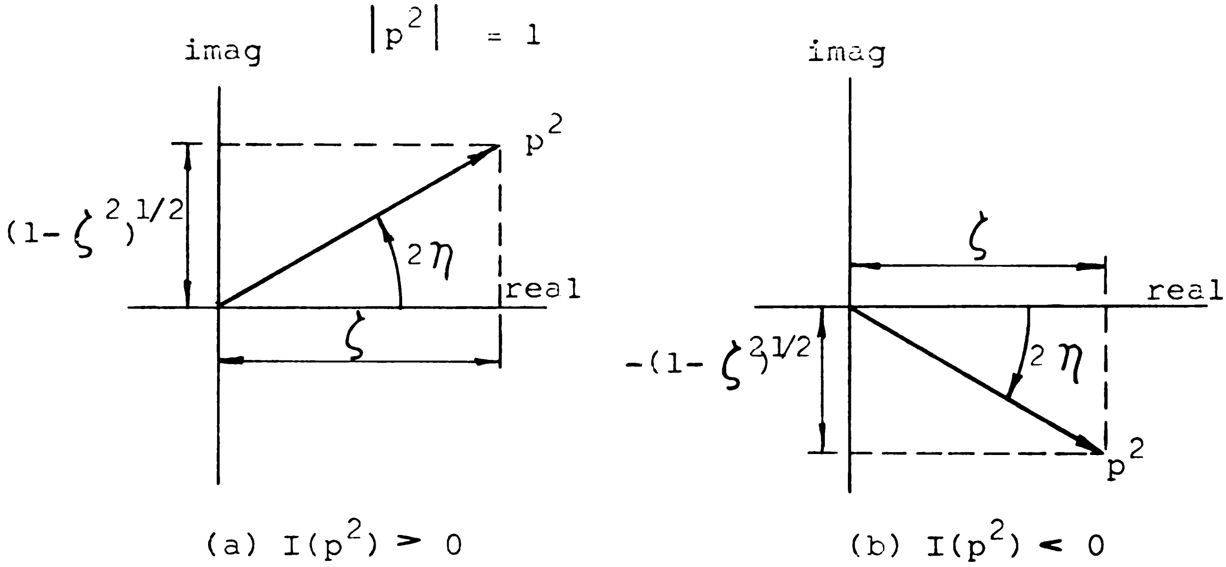


Fig. 30.--Complex representation of p^2

Applying DeMoivre's theorem to equation (9) to find p gives

$$p = \cos(\eta + n\pi) + i\sin(\eta + n\pi).$$

The two independent values of p correspond to n = 0 and n = 1 respectively

$$p_{(1)} = \cos\eta + i\sin\eta \tag{10}$$

$$p_{(2)} = \cos(\eta + \pi) + i\cos(\eta + \pi) = -\cos\eta - i\sin\eta. \tag{11}$$

In exponential form equations (10) and (11) become

$$p_{(1)} = e^{i\eta} \tag{12}$$

$$p_{(2)} = -e^{i\eta}. \tag{13}$$

A similar analysis for the case when p^2 is given by equation (8), with reference to Figure 30b, gives

$$p^2 = \cos(-2\eta + 2n\pi) + i \sin(-2\eta + 2n\pi)$$

$$p = \cos(-\eta + n\pi) + i \sin(-\eta + n\pi).$$

For $n = 0$

$$p_{(3)} = \cos(-\eta) + i \sin(-\eta) = \cos\eta - i \sin\eta. \quad (14)$$

For $n = 1$

$$p_{(4)} = \cos(-\eta + \pi) + i \sin(-\eta + \pi) =$$

$$-\cos\eta + i \sin\eta \quad . \quad (15)$$

Expressing equations (14) and (15) in exponential form gives

$$p_{(3)} = e^{-i\eta} \quad (16)$$

$$p_{(4)} = -e^{-i\eta}. \quad (17)$$

If the constant A_1 is arbitrarily chosen to equal unity the constant A_2, which will henceforth be called A, may be found by solution of either of equations (3) for any one of the four values of p.

$$A_{(i)} = -\frac{c_{11} + c_{44}p_{(i)}^2}{[c_{12} + c_{44}]p_{(i)}} \qquad i = 1, 2, 3, 4 \quad (18)$$

The displacements in equations (2) may now be written as a linear combination of the solutions corresponding to each individual value of p

$$u = f[x + p_{(1)}y] + f[x + p_{(2)}y] + f[x + p_{(3)}y] +$$

$$f[x + p_{(4)}y] \quad (19)$$

$$v = A_{(1)} f[x + p_{(1)} y] + A_{(2)} f[x + p_{(2)} y] + A_{(3)} f[x + p_{(3)} y] + A_{(4)} f[x + p_{(4)} y]. \tag{19}$$

It is noted, however, that $p_{(3)} = e^{-i\eta}$ and $p_{(4)} = -e^{-i\eta}$ are complex conjugates of the values $p_{(1)} = e^{i\eta}$ and $p_{(2)} = -e^{i\eta}$ respectively so that the $f[x + p_{(3)} y]$ and $f[x + p_{(4)} y]$ are complex conjugates of $f[x + p_{(1)} y]$ and $f[x + p_{(2)} y]$ respectively. Similarly, $A_{(3)} f[x + p_{(3)} y]$ and $A_{(4)} f[x + p_{(4)} y]$ are complex conjugates of $A_{(1)} f[x + p_{(1)} y]$ and $A_{(2)} f[x + p_{(2)} y]$ respectively. The imaginary parts of equations (19) will therefore be equal and of opposite sign and will cancel while the real parts are of like sign and will add. (It is physically necessary that u and v be real functions.) In consequence of this only the two roots $p_{(1)} = e^{i\eta}$ and $p_{(2)} = -e^{i\eta}$ will be considered to be independent, and only the functions corresponding to them will be considered in the solution. The imaginary parts of u and v and of any variable derived from u and v, such as stress or strain, will be ignored since they do in fact cancel.

The general form of the displacements for any boundary value problem which satisfies the conditions of plane strain and cubic anisotropy is

$$u = \mathrm{Re}\left\{ f[x + e^{i\eta} y] + f[x - e^{i\eta} y] \right\}$$

$$v = \mathrm{Re}\left\{ A_{(1)} f[x + e^{i\eta} y] + A_{(2)} f[x - e^{i\eta} y] \right\}$$

or

$$u = \mathrm{Re}\left\{f[z_{(1)}] + f[z_{(2)}]\right\}$$

$$v = \mathrm{Re}\left\{A_{(1)}f[z_{(1)}] + A_{(2)}f[z_{(2)}]\right\} \tag{20}$$

where from equation (18)

$$A_{(1)} = -A_{(2)} = -\frac{c_{11}e^{-i\eta} + c_{44}e^{i\eta}}{c_{12} + c_{44}} \tag{21}$$

and

$$\eta = \frac{1}{2}\cos^{-1}\frac{2c_{12}c_{44} + c_{12}^{2} - c_{11}^{2}}{2c_{11}c_{44}}. \tag{22}$$

The form of the function f is determined by the boundary conditions for the specific problem. Consider the case in which the boundary condition involves a displacement discontinuity. The evaluation of the stresses from the displacements in the equations (20) involves expressions of the type

$$\sigma_x = c_{11}\frac{\partial u}{\partial x} + c_{12}\frac{\partial v}{\partial y}.$$

The derivatives in these expressions contain the terms

$$\frac{df[z_{(1)}]}{dz_{(1)}} \quad \text{and} \quad \frac{df[z_{(2)}]}{dz_{(2)}}\ . \tag{23}$$

Because of physical considerations the stresses must be single valued and continuous. This condition will certainly be satisfied if the derivatives of (20) are analytic in those portions of the $z_{(1)}$ and $z_{(2)}$ planes respectively to which the region of interest of the xy plane maps. If these derivatives are analytic in some portion of their respective complex planes, they may be expanded in a power series about some point in the region of analyticity. Suppose that the origin of xy coordinates is the point at which the displacement discontinuity ends. For strictly physical reasons the stresses at this point must be infinite. This point is therefore a singular point in the region. If the point (0,0) is the point of expansion in the $z_{(1)}$ and $z_{(2)}$ planes, the expansions of the derivatives (23) must be of the Laurent type since (0,0) in both these planes is an isolated singularity. Expanding $df[z_{(1)}]/dz_{(1)}$ in a Laurent series about the origin gives

$$\frac{df[z_{(1)}]}{dz_{(1)}} = \ldots + G_{-2}\frac{1}{z_{(1)}^{\;2}} + G_{-1}\frac{1}{z_{(1)}} + G_0 + G_1 z_{(1)} + G_2 z_{(2)} + \ldots \qquad (24)$$

Integrating this expression gives

$$f[z_{(1)}] = \ldots - G_{-2}\frac{1}{z_{(1)}} + G_{-1}\log z_{(1)} + G_0 z_{(1)} + \frac{G_1 z_{(1)}^{\;2}}{2} \ldots \qquad (25)$$

All terms in equation (25) are continuous and single valued in the $z_{(1)}$ plane except the log $z_{(1)}$ term which is infinitely many valued. The many-valued function may be considered a single-valued function by introducing a branch line in the $z_{(1)}$ plane so that no circuit of the origin may cross the branch line. In such a case the value of log $z_{(1)}$ on one side of the branch differs from its value on the other side by the amount $2\pi i$. This discontinuity across the branch line is exactly that property which is necessary to satisfy the discontinuous displacement boundary condition; therefore

$$
\begin{aligned}
f[z_{(1)}] &= G_{-1} \log z_{(1)} = \frac{D_{(1)}}{2\pi i} \log z_{(1)} \\
f[z_{(2)}] &= H_{-1} \log z_{(2)} = \frac{D_{(2)}}{2\pi i} \log z_{(2)}
\end{aligned}
\tag{26}
$$

is chosen for the particular solution.

APPENDIX III

EXPANSION OF LOG $z_{(1)}$ AND LOG $z_{(2)}$ INTO REAL AND IMAGINARY PARTS

Expanding log $z_{(2)}$ into real and imaginary parts gives

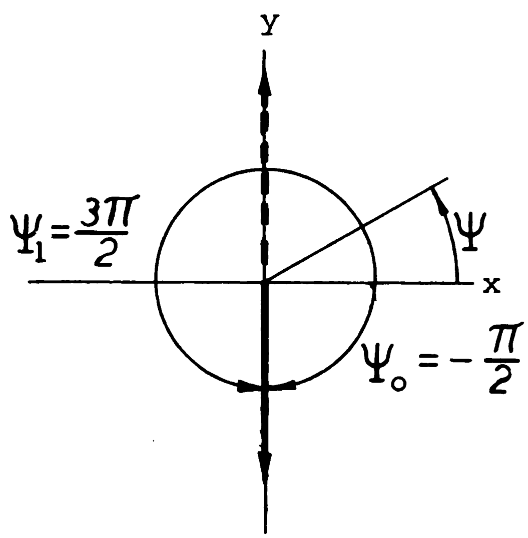
$$w_{(2)} = r_{(2)} + is_{(2)} = \log z_{(2)} = \log (x - e^{i\eta} y) =$$

$$\log (x - y \cos\eta - iy \sin\eta) = \log (x'' + iy'') =$$

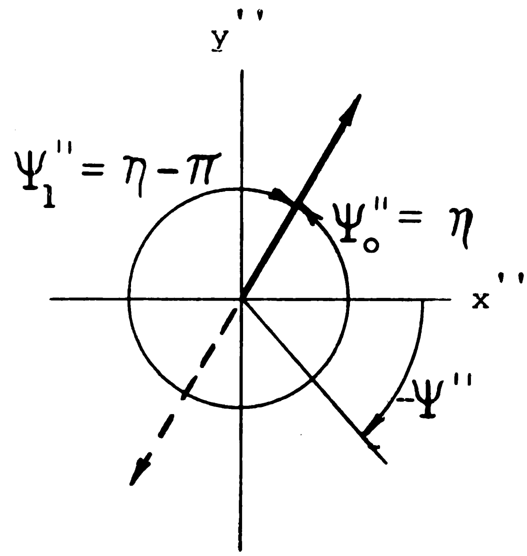
$$\tfrac{1}{2}\log (x''^2 + y''^2) + i[\tan^{-1}(\frac{y''}{x''}) + 2k\pi] = \tfrac{1}{2}\log (x^2 +$$

$$y^2 - 2xy \cos\eta) + i[\tan^{-1}(\frac{-y \sin\eta}{x - y \cos\eta}) + 2k\pi]. \qquad (1)$$

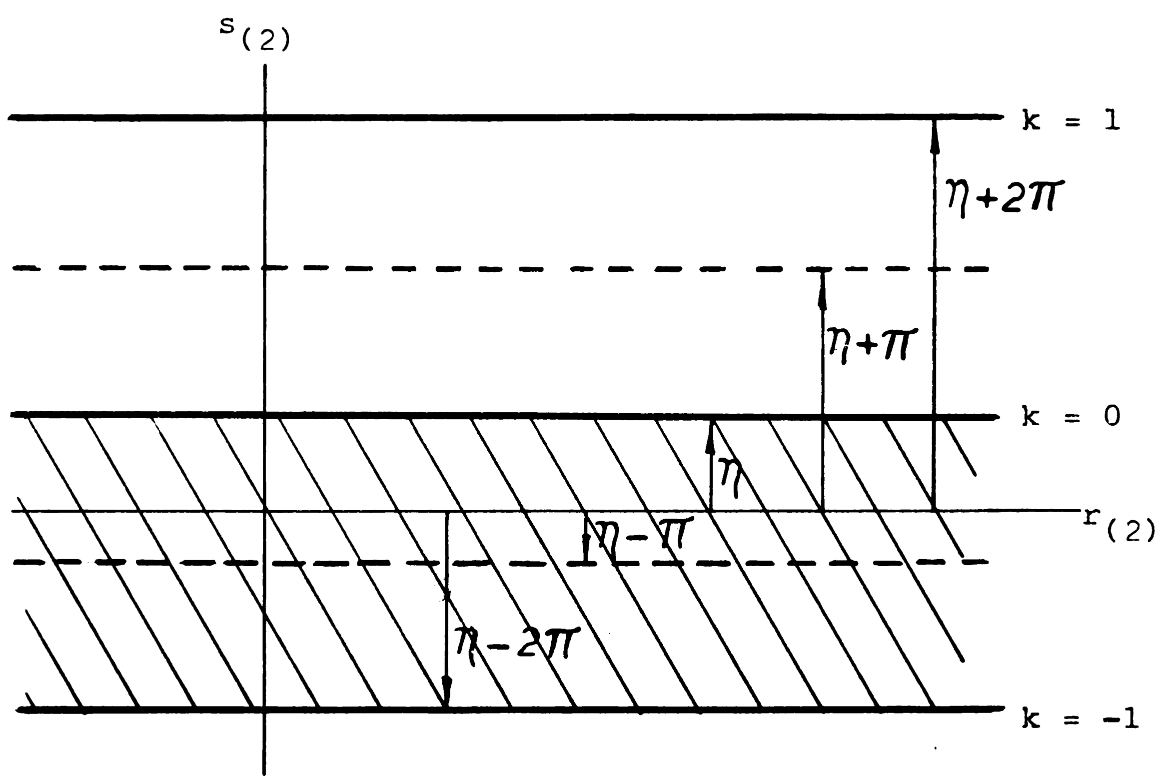
The multivalued log function is being used to represent a single valued but discontinuous displacement. Which branch, then, of the equation (1) will be used to represent the single-valued function? The equation (1) may be thought of as a mapping of the xy plane onto the $x''y''$ plane onto the $r_{(2)}s_{(2)}$ plane. The Figure 31 shows the mapping of the negative y axis from the xy plane to the $x''y''$ plane and then to the $r_{(2)}s_{(2)}$ plane in the heavy black line with the arrow pointing in the direction of increasing absolute value of y. The positive y axis is shown in the dotted black line. Note that increasing Ψ in the xy plane corresponds to decreasing Ψ'' in the $x''y''$ plane. The negative y axis maps onto the infinite



(a) xy plane



(b) x''y'' plane



(c) $r_{(2)}s_{(2)}[w_{(2)}]$ plane

Fig. 31.--Mapping of the xy plane onto the $w_{(2)}$ plane by the function $w_{(2)} = \log z_{(2)}$

number of lines in the $r_{(2)}s_{(2)}$ plane for which

$$s_{(2)} = \Psi'' = \tan^{-1}\frac{\sin\eta}{\cos\eta} + 2k\pi = \eta + 2k\pi.$$

The entire xy plane maps on the strip between any two successive values of k. The mapping may be made single valued by arbitrarily choosing one strip to which the xy plane maps. If the line $\Psi = -\pi/2$ in the xy plane is arbitrarily chosen as corresponding to the line $s_{(2)} = \eta$ $(k = 0)$ in the $r_{(2)}s_{(2)}$ plane, then since Ψ'' decreases as Ψ increases the line $\Psi = 3\pi/2$ in the xy plane corresponds to the line $s_{(2)} = \eta - 2\pi$ $(k = -1)$. The branch of the $r_{(2)}s_{(2)}$ plane to which the xy plane maps is crosshatched in Figure 31.

In a similar manner expand $\log z_{(1)}$

$$w_{(1)} = r_{(1)} + is_{(1)} = \log z_{(1)} = \log(x + e^{i\eta}y) =$$

$$\log(x + y\cos\eta + iy\sin\eta) = \tfrac{1}{2}\log(x'^2 + y'^2) +$$

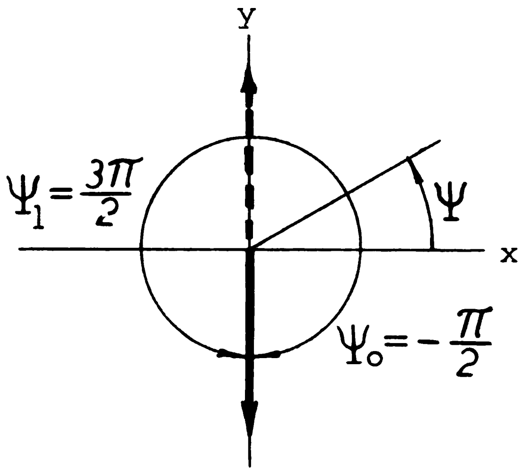
$$i[\tan^{-1}(\frac{y'}{x'}) + 2k\pi] = \tfrac{1}{2}\log(x^2 + y^2 + 2xy\cos\eta) +$$

$$i[\tan^{-1}(\frac{y\sin\eta}{x + y\cos\eta}) + 2k\pi]. \tag{2}$$

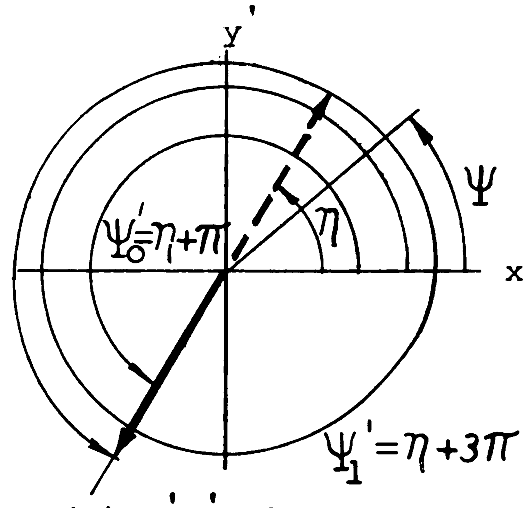
The mapping from the xy plane to the $x'y'$ plane to the $r_{(1)}s_{(1)}$ plane is shown in Figure 32. Here an increasing Ψ corresponds to increasing Ψ'. The negative y axis is mapped onto the infinite number of horizontal lines

$$s_{(1)} = \Psi_0' = \tan^{-1}\frac{-\sin}{-\cos} + 2k\pi = \eta + \pi + 2k\pi$$

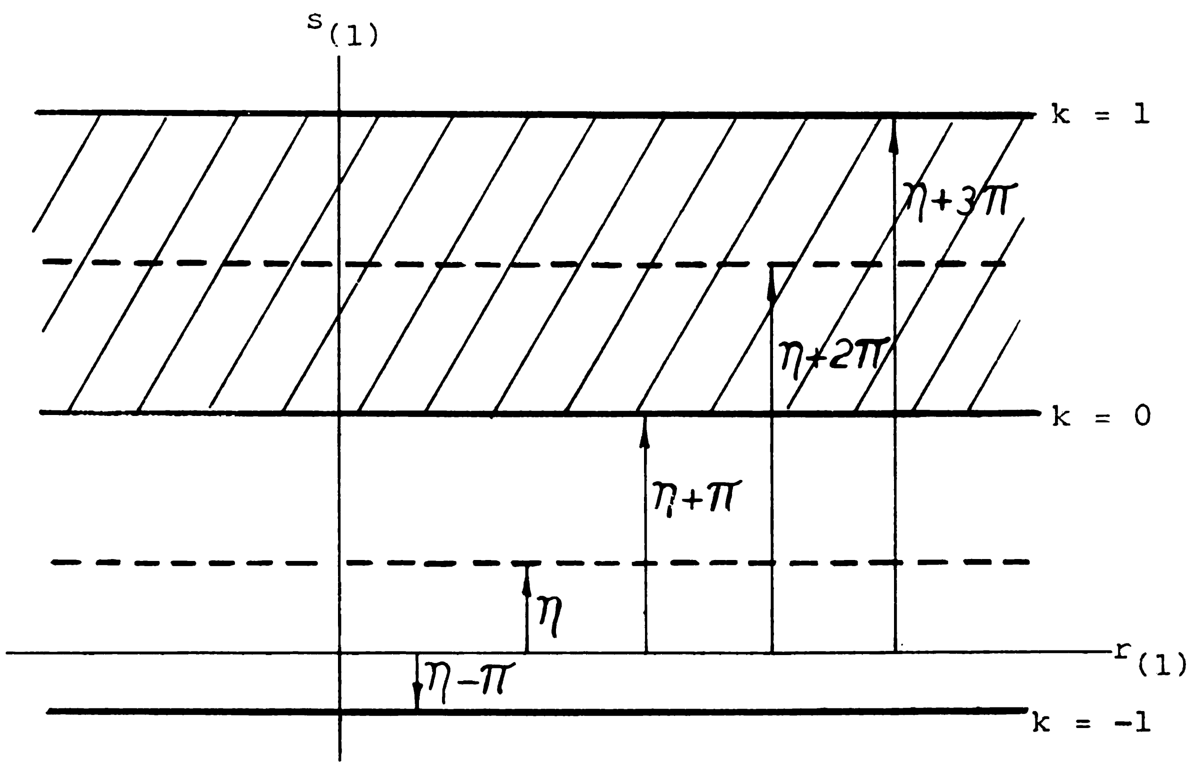
and the entire xy plane maps onto the horizontal strip



(a) xy plane



(b) x'y' plane



(c) $r_{(1)} s_{(1)} [w_{(1)}]$ plane

Fig. 32.--Mapping of xy plane on the $w_{(1)}$ plane by the function $w_{(1)} = \log z_{(1)}$

between any two successive values of k. To make the mapping single valued the line $\Psi = -\pi/2$ in the xy plane will be arbitrarily chosen to correspond to $s_{(1)} = \eta + \pi$ $(k = 0)$ in the $r_{(1)}s_{(1)}$ plane in which case the line $\Psi = 3\pi/2$ corresponds to the line $s_{(1)} = \eta + 3\pi$ $(k = 1)$ since increasing Ψ corresponds to increasing Ψ'. The branch between k = 0 and k = 1 is crosshatched in Figure 32.

As an example of the evaluation of the functions $\log z_{(1)}$ and $\log z_{(2)}$, find the points in the $z_{(1)}$ and $z_{(2)}$ planes to which the point $x = .5$ and $y = -.25$ maps, for the case

$$\sin\eta = .790569$$
$$\cos\eta = .612372$$
$$\eta = .911738.$$

These values correspond to the case $c_{12} = c_{44} = c_{11}/2$.

$$\log z_{(1)} = r_{(1)} + is_{(1)}$$

$$r_{(1)} = \tfrac{1}{2}\log(x^2 + y^2 + 2xy\cos\eta) = \tfrac{1}{2}\log[.25 + .0625 + 2(.5)(-.25)(.61237)]$$

$$r_{(1)} = \tfrac{1}{2}\log(.15841) = \tfrac{1}{2}(-1.84256) = -.92128$$

$$\tan\ ' = \frac{y \sin}{x + y \cos} = \frac{-.25(.79057)}{.5 - .25(.61237)} = \frac{-.79057}{1.38763}$$

$$\tan\Psi' = -.56973$$

This angle Ψ' is in the fourth quadrant of the $x'y'$ plane

$$\Psi' = -.51787 \text{ rad}$$

$$s_{(1)} = 2\pi - .51787 = 6.28319 - .51787 = 5.76532 \text{ rad}$$

$\log z_{(1)} = -.92128 + 5.76532i$

$\log z_{(2)} = r_{(2)} + is_{(2)}$

$r_{(2)} = \frac{1}{2}\log(x^2 + y^2 - 2xy \cos\eta) = \frac{1}{2}\log[.25 + .0625 -$

$2(.5)(-.25)(.61237)] = \frac{1}{2}\log(.46659) = \frac{1}{2}(-.76232) =$

$-.38116$

$$\tan\Psi'' = \frac{y \sin}{x - y \cos} = \frac{-(-.25)(.79057)}{.5 - (-.25)(.61237)} = \frac{.79057}{2.61237}$$

$\tan\Psi'' = .30263$

The angle Ψ'' lies in the first quadrant of the $x''y''$ plane

$\Psi'' = .29387$ rad

$s_{(2)} = .29387$

$\log z_{(2)} = -.38116 + .29387i.$

APPENDIX IV

SIMILARITY OF DISCRETE AND CONTINUUM MODELS

The response of the discrete material model to mechanical disturbance is characterized by the constants α and β, while the response of the continuum model is determined by the constants c_{11}, c_{12}, and c_{44}. In order to compare the response of these two models to the same type of stimulus these models must be made in some sense similar. Depending on how this similarity is defined a relationship will exist between the constants of the two models. The similarity between the two models will now be defined and the relationships between the two sets of constants will be determined.

Following the example of Kittel [10] consider the x component of the force equilibrium equation for an atom which is surrounded by a normal complement of neighbors.

$$\alpha(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) + \frac{\beta}{2}(u_{i+1,j+1} - 2u_{i,j} + u_{i-1,j-1}) + \frac{\beta}{2}(v_{i+1,j+1} - 2v_{i,j} + v_{i-1,j-1}) + \frac{\beta}{2}(u_{i-1,j+1} - 2u_{i,j} + u_{i+1,j-1}) - \frac{\beta}{2}(v_{i-1,j+1} - 2v_{i,j} + v_{i+1,j-1}) = 0 \tag{1}$$

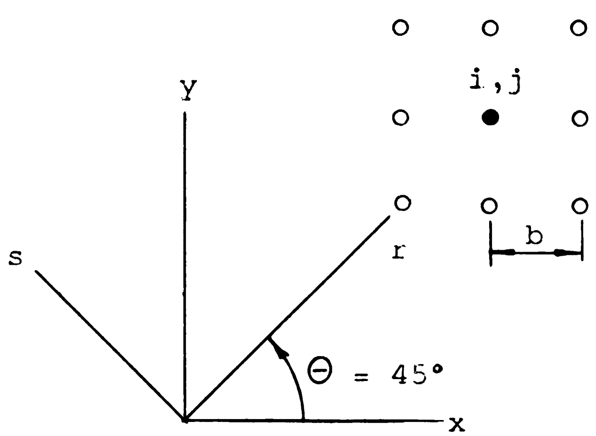
This equation is the same as the equation (2.10) except that several terms which cancel have been retained and the grouping of terms is different. Suppose now that the atomic displacement, b, is allowed to approach zero. The difference equation (1) then passes to the differential equation

$$b^2\alpha \frac{\partial^2 u}{\partial x^2} + 2b^2 \frac{\beta}{2} \frac{\partial^2 u}{\partial r^2} + 2b^2 \frac{\beta}{2} \frac{\partial^2 v}{\partial r^2} + 2b^2 \frac{\beta}{2} \frac{\partial^2 u}{\partial s^2} -$$

$$2b^2 \frac{\beta}{2} \frac{\partial^2 v}{\partial s^2} = 0. \tag{2}$$

The variables r and s and the difference approximations for the second derivatives are shown in Figure 33.

The derivatives with respect to r and s in equation (2) may be replaced by derivatives with respect



$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \simeq \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{b^2}$$

$$\left(\frac{\partial^2 u}{\partial r^2}\right)_{i,j} \simeq \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{b^2}$$

$$\left(\frac{\partial^2 u}{\partial s^2}\right)_{i,j} \simeq \frac{u_{i-1,j+1} - 2u_{i,j} + u_{i+1,j-1}}{b^2}$$

Fig. 33.--Relation of (x,y) coordinate to (r,s) coordinates

to x and y by using the following transformation:

$$\frac{\partial u}{\partial r} = \frac{\partial u}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial r}$$

$$\frac{\partial^2 u}{\partial r^2} = \frac{\partial x}{\partial r}\frac{\partial}{\partial r}\left(\frac{\partial u}{\partial x}\right) + \frac{\partial u}{\partial x}\frac{\partial^2 x}{\partial r^2} + \frac{\partial y}{\partial r}\frac{\partial}{\partial r}\left(\frac{\partial u}{\partial y}\right) + \frac{\partial u}{\partial y}\frac{\partial^2 y}{\partial r^2}. \qquad (3)$$

Noting that

$$\frac{\partial}{\partial r}\left(\frac{\partial u}{\partial x}\right) = \frac{\partial^2 u}{\partial x^2}\frac{\partial x}{\partial r} + \frac{\partial^2 u}{\partial x \partial y}\frac{\partial y}{\partial r}$$

and

$$\frac{\partial}{\partial r}\left(\frac{\partial u}{\partial y}\right) = \frac{\partial^2 u}{\partial x \partial y}\frac{\partial x}{\partial r} + \frac{\partial^2 u}{\partial y^2}\frac{\partial y}{\partial r}$$

and then substituting into equation (3) gives

$$\frac{\partial^2 u}{\partial r^2} = \frac{\partial^2 u}{\partial x^2}\left(\frac{\partial x}{\partial r}\right)^2 + \frac{\partial^2 u}{\partial x \partial y}\frac{\partial x}{\partial r}\frac{\partial y}{\partial r} + \frac{\partial u}{\partial x}\frac{\partial^2 x}{\partial r^2} + \frac{\partial^2 u}{\partial x \partial y}\frac{\partial x}{\partial r}\frac{\partial y}{\partial r} + \frac{\partial^2 u}{\partial y^2}\left(\frac{\partial y}{\partial r}\right)^2 + \frac{\partial u}{\partial y}\frac{\partial^2 y}{\partial r^2}. \qquad (4)$$

The relationships between r,s and x,y are

$$x = r\cos\Theta$$

$$y = r\sin\Theta$$

so that

$$\frac{\partial x}{\partial r} = \cos\Theta$$

$$\frac{\partial y}{\partial r} = \sin\Theta$$

$$\frac{\partial^2 x}{\partial r^2} = \frac{\partial^2 y}{\partial r^2} = 0.$$

Substitution of these derivatives into equation (4) gives

$$\frac{\partial^2 u}{\partial r^2} = \cos^2\Theta \frac{\partial^2 u}{\partial x^2} + 2\sin\Theta\cos\Theta \frac{\partial^2 u}{\partial x \partial y} + \sin^2\Theta \frac{\partial^2 u}{\partial y^2} \tag{5}$$

and for $\Theta = 45°$ this equation becomes

$$\frac{\partial^2 u}{\partial r^2} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial x \partial y} + \frac{1}{2}\frac{\partial^2 u}{\partial y^2} . \tag{6}$$

In a similar manner since

$$x = -s\sin\Theta \qquad \frac{\partial x}{\partial s} = -\sin\Theta$$

$$y = s\cos\Theta \qquad \frac{\partial y}{\partial s} = \cos\Theta$$

$$\frac{\partial^2 u}{\partial s^2} = \sin^2\Theta \frac{\partial^2 u}{\partial x^2} - 2\sin\Theta\cos\Theta \frac{\partial^2 u}{\partial x \partial y} + \cos^2\Theta \frac{\partial^2 u}{\partial y^2}$$

and for $\Theta = 45°$

$$\frac{\partial^2 u}{\partial s^2} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial x \partial y} + \frac{1}{2}\frac{\partial^2 u}{\partial x^2} . \tag{7}$$

Equation (2) may now be rewritten in terms of x and y derivatives as

$$b^2\alpha \frac{\partial^2 u}{\partial x^2} + b^2\beta\left(\frac{1}{2}\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial x \partial y} + \frac{1}{2}\frac{\partial^2 u}{\partial y^2}\right) + b^2\beta\left(\frac{1}{2}\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial x \partial y} + \frac{1}{2}\frac{\partial^2 v}{\partial x^2}\right) + b^2\beta\left(\frac{1}{2}\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial x \partial y} + \frac{1}{2}\frac{\partial^2 u}{\partial y^2}\right) - b^2\beta\left(\frac{1}{2}\frac{\partial^2 v}{\partial x^2} - \frac{\partial^2 v}{\partial x \partial y} + \frac{1}{2}\frac{\partial^2 v}{\partial y^2}\right) = 0.$$

This simplifies to

$$b^2(\alpha + \beta)\frac{\partial^2 u}{\partial x^2} + b^2\beta \frac{\partial^2 u}{\partial y^2} + 2b^2\beta \frac{\partial^2 v}{\partial x \partial y} = 0. \tag{8}$$

The x component of the static equilibrium equation for plane strain in an elastic continuum with cubic anisotropy is

$$c_{11} \frac{\partial^2 u}{\partial x^2} + c_{44} \frac{\partial^2 u}{\partial y^2} + (c_{12} + c_{44}) \frac{\partial^2 v}{\partial x \partial y} = 0. \tag{9}$$

Dividing equation (8) by b^3 to achieve dimensional similarity and then comparing with equation (9), it may be seen that the two equations are exactly the same if their respective coefficients satisfy the relationships

$$\begin{aligned} c_{11} &= \frac{(\alpha + \beta)}{b} \\ c_{44} &= \frac{\beta}{b} \\ c_{12} + c_{44} &= \frac{2\beta}{b} \\ &\text{or} \\ c_{11} &= \frac{2\beta}{b}. \end{aligned} \tag{10}$$

The condition $c_{12} = c_{44}$ results from the central force assumption for the discrete model [see Kittel]. For the special case $\alpha = \beta$

$$c_{11}/2 = c_{12} = c_{44}. \tag{11}$$

It should be noted that the relationships (10) and (11) do not conform to those which describe an isotropic solid. In Love [1] it is shown that the relationship between the elastic constants for an isotropic material is

$$c_{44} = \frac{1}{2}(c_{11} - c_{12}). \tag{12}$$

But by the relationship (10) c_{12} must equal c_{44}; therefore

$$c_{12} = \frac{1}{2}(c_{11} - c_{12})$$

or

$$c_{11} = 3c_{12}.$$

Substituting this relationship into equations (10) gives

$$3c_{12} = (\alpha + \beta)/b$$

$$c_{12} = \beta/b$$

$$3\beta/b = (\alpha + \beta)/b$$

$$2\beta = \alpha. \qquad (13)$$

Therefore for a central force model elastic isotropy corresponds to the specific relationship (13) between the discrete force constants α and β.

APPENDIX V

FORM OF THE STRESS FUNCTION EQUATION

In Chapter III it is shown that for the case of plane strain a function ϕ exists such that

$$\sigma_x = \frac{\partial^2 \phi}{\partial y^2}$$

$$\sigma_y = \frac{\partial^2 \phi}{\partial x^2}$$

$$\tau_{xy} = -\frac{\partial^2 \phi}{\partial x \partial y} .$$

Expressing the stresses in terms of displacements leads to the equations

$$c_{11} \frac{\partial u}{\partial x} + c_{12} \frac{\partial v}{\partial y} = \frac{\partial^2 \phi}{\partial y^2} \tag{1}$$

$$c_{11} \frac{\partial v}{\partial y} + c_{12} \frac{\partial u}{\partial x} = \frac{\partial^2 \phi}{\partial x^2} \tag{2}$$

$$c_{44}\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) = -\frac{\partial^2 \phi}{\partial x \partial y} \tag{3}$$

for the case of cubic anisotropy. Solving equations (1) and (2) for $\partial u/\partial x$ and $\partial v/\partial y$ gives

$$\frac{\partial u}{\partial x} = \frac{c_{11}}{c_{11}^2 - c_{12}^2} \frac{\partial^2 \phi}{\partial y^2} - \frac{c_{12}}{c_{11}^2 - c_{12}^2} \frac{\partial^2 \phi}{\partial x^2} \tag{4}$$

$$\frac{\partial v}{\partial y} = \frac{c_{11}}{c_{11}^2 - c_{12}^2} \frac{\partial^2 \phi}{\partial x^2} - \frac{c_{12}}{c_{11}^2 - c_{12}^2} \frac{\partial^2 \phi}{\partial y^2} . \tag{5}$$

Differentiating equation (3) with respect to both x and y gives

$$\frac{\partial^3 u}{\partial x \partial y^2} + \frac{\partial^3 v}{\partial y \partial x^2} = -\frac{1}{c_{44}} \frac{\partial^4 \phi}{\partial x^2 \partial y^2} . \tag{6}$$

Now differentiate equation (4) twice with respect to y and differentiate equation (5) twice with respect to x

$$\frac{\partial^3 u}{\partial x \partial y^2} = \frac{c_{11}}{c_{11}^2 - c_{12}^2} \frac{\partial^4 \phi}{\partial y^4} - \frac{c_{12}}{c_{11}^2 - c_{12}^2} \frac{\partial^4 \phi}{\partial x^2 \partial y^2} \tag{7}$$

$$\frac{\partial^3 u}{\partial y \partial x^2} = \frac{c_{11}}{c_{11}^2 - c_{12}^2} \frac{\partial^4 \phi}{\partial x^4} - \frac{c_{12}}{c_{11}^2 - c_{12}^2} \frac{\partial^4 \phi}{\partial x^2 \partial y^2} . \tag{8}$$

Substitute the two third mixed partial derivatives (7) and (8) into equation (6)

$$\frac{c_{11}}{c_{11}^2 - c_{12}^2} \frac{\partial^4 \phi}{\partial y^4} - \frac{c_{12}}{c_{11}^2 - c_{12}^2} \frac{\partial^4 \phi}{\partial x^2 \partial y^2} + \frac{c_{11}}{c_{11}^2 - c_{12}^2} \frac{\partial^4 \phi}{\partial x^4} - \frac{c_{12}}{c_{11}^2 - c_{12}^2} \frac{\partial^4 \phi}{\partial x^2 \partial y^2} = -\frac{1}{c_{44}} \frac{\partial^4 \phi}{\partial x^2 \partial y^2} . \tag{9}$$

Simplification of this equation gives the partial differential equation, commonly known as the compatibility equation, which the function ϕ must satisfy for the case of cubic symmetry

$$c_{11} \frac{\partial^4 \phi}{\partial x^2} + \frac{c_{11}^2 - 2c_{12}c_{44} - c_{12}^2}{c_{44}} \frac{\partial^4 \phi}{\partial x^2 \partial y^2} + \frac{c_{11} \partial^4 \phi}{\partial y^2} = 0. \tag{10}$$

APPENDIX VI

CALCULATION OF THE BOUNDARY VALUES OF ϕ FOR THE NUMERICAL SOLUTION

On the top boundary $y_1 = 1$

$$\sigma_y = \frac{b}{L} C_2 \frac{(x_1^{\,2} - 1)}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\tau_{xy} = \frac{b}{L} C_2 \frac{(x_1^{\,3} - x_1)}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\frac{1}{L^2} \frac{\partial^2 \phi}{\partial x_1 \partial y_1} = - \tau_{xy} = \frac{b}{L} C_2 \frac{(x_1 - x_1^{\,3})}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\frac{\partial^2 \phi}{\partial x_1 \partial y_1} = bLC_2 \frac{x_1 - x_1^{\,3}}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\frac{\partial \phi}{\partial y_1} = bL \left[C_2 \frac{(1 + .5D)}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2x_1^{\,2} + D}{(4 - D^2)^{1/2}} - .25C_2 \log(x_1^{\,4} + Dx_1^{\,2} + 1) + K_1 \right] \qquad (1)$$

$$\frac{1}{L^2} \frac{\partial^2 \phi}{\partial x_1^{\,2}} = \sigma_y = \frac{b}{L} C_2 \frac{(x_1^{\,2} - 1)}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\frac{\partial^2 \phi}{\partial x_1^{\,2}} = bLC_2 \frac{(x_1^{\,2} + 1)}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\frac{\partial \phi}{\partial x_1} = bL \left[\frac{.25C_2}{\cos \eta} \log \frac{x_1^{\,2} - 2x_1 \cos \eta + 1}{x_1^{\,2} + 2x_1 \cos \eta + 1} + K_2 \right] \qquad (2)$$

$$\phi = bL\left[\frac{.25C_2}{\cos\eta}\,x_1\,\log\frac{x_1^{\;2} - 2x_1\,\cos\eta + 1}{x_1^{\;2} + 2x_1\,\cos\eta + 1} - .25C_2\right.$$

$$\log(x_1^{\;4} + Dx_1^{\;2} + 1) + C_2\,\frac{(1 + .5D)}{(4 - D^2)^{1/2}}\,\tan^{-1}$$

$$\left.\frac{2x_1^{\;2} + D}{(4 - D^2)^{1/2}} + K_2x_1 + K_3\right]. \tag{3}$$

On the side boundary $x_1 = 1$

$$\frac{1}{L^2}\,\frac{\partial^2\phi}{\partial x_1\,\partial y_1} = -\tau_{xy} = \frac{b}{L}\,C_2\,\frac{y_1^{\;2} - 1}{y_1^{\;4} + Dy_1^{\;2} + 1}$$

$$\frac{\partial^2\phi}{x_1\quad y_1} = bLC_2\,\frac{y_1^{\;2} - 1}{y_1^{\;4} + Dy_1^{\;2} + 1}$$

$$\frac{\partial\phi}{\partial x_1} = bL\left[\frac{.25C_2}{\cos\eta}\,\log\frac{y_1^{\;2} - 2y_1\,\cos\eta + 1}{y_1^{\;2} + 2y_1\,\cos\eta + 1} + K_4\right] \tag{4}$$

$$\frac{1}{L^2}\,\frac{\partial^2\phi}{\partial y_1^{\;2}} = \sigma_x = \frac{b}{L}\,\frac{-C_1y_1 - C_2y_1^{\;3}}{y_1^{\;4} + Dy_1^{\;2} + 1}$$

$$\frac{\partial^2\phi}{\partial y_1^{\;2}} = bL\,\frac{-C_1y_1 - C_2y_1^{\;3}}{y_1^{\;4} + Dy_1^{\;2} + 1}$$

$$\frac{\partial\phi}{\partial y_1} = bL\left[\frac{-C_1 + .5DC_2}{(4 - D^2)^{1/2}}\,\tan^{-1}\frac{2y_1^{\;2} + D}{(4 - D^2)^{1/2}} - .25C_2\right.$$

$$\left.\log(y_1^{\;4} + Dy_1^{\;2} + 1) + K_5\right] \tag{5}$$

$$\phi = bL\left[\frac{-C_1 + .5DC_2}{(4 - D^2)^{1/2}} y_1 \tan^{-1} \frac{2y_1^{\,2} + D}{(4 - D^2)^{1/2}} - .25C_2 y_1 \right.$$

$$\log(y_1^{\,4} + Dy_1^{\,2} + 1) + \frac{(DC_2 - C_1 - C_2)}{8 \cos\eta}$$

$$\log \frac{y_1^{\,2} + 2\cos\eta\, y_1 + 1}{y_1^{\,2} - 2\cos\eta\, y_1 + 1} - \frac{(C_2 + C_2 D - C_1)}{4 \sin\eta} \tan^{-1}$$

$$\left. \frac{2y_1 \sin\eta}{1 - y_1^{\,2}} + C_2 y_1 + K_5 y_1 + K_6 \right]. \qquad (6)$$

On the bottom boundary $y_1 = -1$

$$\frac{1}{L^2} \frac{\partial^2 \phi}{\partial x_1 \partial y_1} = -\tau_{xy} = \frac{b}{L} C_2 \frac{x_1 - x_1^{\,3}}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\frac{\partial^2 \phi}{\partial x_1 \partial y_1} = bLC_2 \frac{x_1 - x_1^{\,2}}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\frac{\partial \phi}{\partial y_1} = bL\left[C_2 \frac{(1 + .5D)}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2x_1^{\,2} + D}{(4 - D^2)^{1/2}} - .25C_2 \right.$$

$$\left. \log(x_1^{\,4} + Dx_1^{\,2} + 1) + K_7 \right] \qquad (7)$$

$$\frac{1}{L^2} \frac{\partial^2 \phi}{\partial x_1^{\,2}} = \sigma_y = \frac{b}{L} C_2 \frac{1 - x_1^{\,2}}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\frac{\partial^2 \phi}{\partial x_1^{\,2}} = bLC_2 \frac{1 - x_1^{\,2}}{x_1^{\,4} + Dx_1^{\,2} + 1}$$

$$\frac{\partial \phi}{\partial x_1} = bL\left[\frac{-.25C_2}{\cos\eta} \log \frac{x_1^{\,2} - 2x_1 \cos\eta + 1}{x_1^{\,2} + 2x_1 \cos\eta + 1} + K_8\right] \qquad (8)$$

$$\phi = bL\left[\frac{-.25C_2}{\cos\eta} x_1 \log\frac{x_1{}^2 - 2x_1\cos\eta + 1}{x_1{}^2 + 2x_1\cos\eta + 1} + .25C_2\right.$$

$$\log(x_1{}^4 + Dx_1{}^2 + 1) - C_2\frac{(1 + .5D)}{(4 - D^2)^{1/2}}\tan^{-1}\frac{2x_1{}^2 + D}{(4 - D^2)^{1/2}} +$$

$$\left.K_8x_1 + K_9\right]. \tag{9}$$

If ϕ is to be symmetrical with respect to $x_1 = 0$ the constant K_2 must be taken as zero. The constants K_1 and K_3 are arbitrarily set equal to zero. All other integration constants may now be found from the continuity requirement at the two corners.

Equate $\frac{\partial\phi}{\partial x_1}$ from the top and side boundaries at the intersection of these boundaries

$$\frac{.25C_2}{\cos\eta}\log\frac{1 - \cos\eta}{1 + \cos\eta} = \frac{.25C_2}{\cos\eta}\log\frac{1 - \cos\eta}{1 + \cos\eta} + K_4$$

$$K_4 = 0. \tag{10}$$

Equate $\frac{\partial\phi}{\partial y_1}$ at the top corner

$$\frac{-C_1 + .5DC_2}{(4 - D^2)^{1/2}}\tan^{-1}\frac{2 + D}{(4 - D^2)^{1/2}} - .25C_2\log(2 + D) + K_5 =$$

$$\frac{C_2 + .5DC_2}{(4 - D^2)^{1/2}}\tan^{-1}\frac{2 + D}{(4 - D^2)^{1/2}} - .25C_2\log|2 + D|$$

$$K_5 = \frac{C_1 + C_2}{(4 - D^2)^{1/2}}\tan^{-1}\frac{2 + D}{(4 - D^2)^{1/2}}. \tag{11}$$

Equate ϕ at the top corner

$$\frac{-C_1 + .5DC_2}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2 + D}{(4 - D^2)^{1/2}} - .25C_2 \log (2 + D) +$$

$$\frac{(DC_2 - C_1 - C_2)}{8 \cos\eta} \log \frac{1 + \cos\eta}{1 - \cos\eta} - \frac{(C_2 + C_2D - C_1)}{4 \sin\eta} \frac{\pi}{2} +$$

$$C_2 + \frac{C_1 + C_2}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2 + D}{(4 - D^2)^{1/2}} + K_6 = \frac{.25C_2}{\cos\eta}$$

$$\log \frac{1 - \cos\eta}{1 + \cos\eta} - .25C_2 \log \frac{1 - \cos\eta}{1 + \cos\eta} + \frac{C_2 + .5C_2D}{(4 - D^2)^{1/2}}$$

$$\tan^{-1} \frac{2 + D}{(4 - D^2)^{1/2}}$$

$$K_6 = \frac{C_2 + DC_2 - C_1}{8 \cos\eta} \log \frac{1 - \cos\eta}{1 + \cos\eta} +$$

$$\frac{C_2 + C_2D - C_1}{4 \sin\eta} \frac{\pi}{2} - C_2. \qquad (12)$$

Equate $\frac{\partial \phi}{\partial x_1}$ at the lower corner

$$\frac{-.25C_2}{\cos\eta} \log \frac{1 - \cos\eta}{1 + \cos\eta} + K_8 = \frac{.25C_2}{\cos\eta} \frac{1 + \cos\eta}{1 - \cos\eta}$$

$$K_8 = 0. \qquad (13)$$

Equate $\frac{\partial \phi}{\partial Y_1}$ at lower corner

$$\frac{C_2 + .5DC_2}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2 + D}{(4 - D^2)^{1/2}} - .25C_2 \log(2 + D) + K_7 =$$

$$\frac{-C_1 + .5DC_2}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2 + D}{(4 - D^2)^{1/2}} - .25C_2 \log(2 + D) +$$

$$\frac{C_1 + C_2}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2 + D}{(4 - D^2)^{1/2}}$$

$$K_7 = 0. \qquad (14)$$

Equate ϕ at the lower corner

$$\frac{-.25C_2}{\cos\eta} \log \frac{1 - \cos\eta}{1 + \cos\eta} + .25C_2 \log(2 + D) - \frac{C_2 + .5DC_2}{(4 - D^2)^{1/2}}$$

$$\tan^{-1} \frac{2 + D}{(4 - D^2)^{1/2}} + K_9 = - \frac{-C_1 + .5DC_2}{(4 - D^2)^{1/2}} \tan^{-1}$$

$$\frac{2 + D}{(4 - D^2)^{1/2}} + .25C_2 \log(2 + D) + \frac{(DC_2 - C_1 - C_2)}{8 \cos\eta}$$

$$\log \frac{1 - \cos\eta}{1 + \cos\eta} - \frac{(C_2 + C_2D - C_1)}{4 \sin\eta} \left(- \frac{\pi}{2}\right) - C_2 -$$

$$\frac{C_1 + C_2}{(4 - D^2)^{1/2}} \tan^{-1} \frac{2 + D}{(4 - D^2)^{1/2}} + \frac{C_2 + DC_2 - C_1}{8 \cos\eta}$$

$$\log \frac{1 - \cos\eta}{1 + \cos\eta} + \frac{C_2 + C_2D - C_1}{4 \cos\eta} \left(\frac{\pi}{2}\right) - C_2$$

$$K_9 = \frac{C_2 + DC_2 - C_1}{4 \cos\eta} \log \frac{1 - \cos}{1 + \cos} +$$

$$\frac{C_2 + C_2D - C_1}{4 \sin\eta} \pi - 2C_2. \tag{15}$$

APPENDIX VII

THE SYSTEM OF FINITE DIFFERENCE EQUATIONS

Referring to Figure 14, the system of finite difference equations for the rectangular region with boundary tractions given by equations 3.66 through 3.71 with δ = .125 is shown below

$i = 1,\ j = 1$

$$15\phi_{1,1} - 10\phi_{2,1} - 5\phi_{1,2} + 2\phi_{3,1} + \phi_{1,3} + \phi_{2,2} = B_{1,1}$$

$i = 2,\ j = 1$

$$16\phi_{2,1} - 5(\phi_{3,1} + \phi_{2,2} + \phi_{1,1}) + \phi_{4,1} + \phi_{2,3} + .5(\phi_{3,2} + \phi_{1,2}) = B_{2,1}$$

$3 \leq i \leq 6,\ j = 1$

$$15\phi_{i,1} - 5(\phi_{i+1,1} + \phi_{i-1,1} + \phi_{i,2}) + \phi_{i+2,1} + \phi_{i-2,1} + \phi_{i,3} + .5(\phi_{i+1,2} + \phi_{i-1,2}) = B_{i,1}$$

$i = 7,\ j = 1$

$$15\phi_{7,1} - 5(\phi_{8,1} + \phi_{7,2} + \phi_{6,1}) + \phi_{5,1} + \phi_{7,3} + .5(\phi_{8,2} + \phi_{6,2}) = B_{7,1}$$

$i = 8,\ j = 1$

$$16\phi_{8,1} - 5(\phi_{8,2} + \phi_{7,1}) + \phi_{8,3} + \phi_{6,1} + .5\phi_{7,2} = B_{8,1}$$

$i = 1,\ j = 2$

$$14\phi_{1,2} - 10\phi_{2,2} - 5(\phi_{1,3} + \phi_{1,1}) + 2\phi_{3,2} + \phi_{1,4} + \phi_{3,3} + \phi_{3,1} = B_{1,2}$$

$i = 2,\ j = 2$

$$15\phi_{2,2} - 5(\phi_{3,2} + \phi_{1,2} + \phi_{2,3} + \phi_{2,1}) + \phi_{4,2} + \phi_{2,4} + .5(\phi_{3,1} + \phi_{3,3} + \phi_{1,1} + \phi_{1,3}) = B_{2,2}$$

$3 \le i \le 6,\ j = 2$

$$14\phi_{i,2} - 5(\phi_{i+1,2} + \phi_{i-1,2} + \phi_{i,3} + \phi_{i,1}) + \phi_{i+2,2} + \phi_{i-2,2} + \phi_{i,4} + .5(\phi_{i+1,3} + \phi_{i+1,1} + \phi_{i-1,3} + \phi_{i-1,1}) = B_{i,2}$$

$i = 7,\ j = 2$

$$14\phi_{7,2} - 5(\phi_{8,2} + \phi_{6,2} + \phi_{7,3} + \phi_{7,1}) + \phi_{5,2} + \phi_{7,4} + .5(\phi_{8,3} + \phi_{8,1} + \phi_{6,3} + \phi_{6,1}) = B_{7,2}$$

$i = 8,\ j = 2$

$$15\phi_{8,2} - 5(\phi_{7,2} + \phi_{8,3} + \phi_{8,1}) + \phi_{6,2} + \phi_{8,4} + .5(\phi_{7,3} + \phi_{7,1}) = B_{8,2}$$

$i = 1,\ 3 \le j \le 13$

$$14\phi_{1,j} - 10\phi_{2,j} - 5(\phi_{1,j+1} + \phi_{1,j-1}) + 2\phi_{3,j} + \phi_{1,j+2} + \phi_{1,j-2} + \phi_{2,j+1} + \phi_{2,j-1} = 0$$

$i = 2, \; 3 \leq j \leq 13$

$$15\phi_{2,j} - 5(\phi_{3,j} + \phi_{1,j} + \phi_{2,j+1} + \phi_{2,j-1}) + \phi_{4,j} + \phi_{2,j+2} + \phi_{1,j-2} + .5(\phi_{3,j+1} + \phi_{3,j-1} + \phi_{1,j+1} + \phi_{1,j-1}) = 0$$

$3 \leq i \leq 6, \; 3 \leq j \leq 13$

$$14\phi_{i,j} - 5(\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1}) + \phi_{i+2,j} + \phi_{i-2,j} + \phi_{i,j+2} + \phi_{i,j-2} + .5(\phi_{i+1,j+1} + \phi_{i+1,j-1} + \phi_{i-1,j+1} + \phi_{i-1,j-1}) = 0$$

$i = 7, \; 3 \leq j \leq 13$

$$14\phi_{7,j} - 5(\phi_{8,j} + \phi_{6,j} + \phi_{7,j+1} + \phi_{7,j-1}) + \phi_{7,j+2} + \phi_{7,j-2} + \phi_{5,j} + .5(\phi_{8,j+1} + \phi_{8,j-1} + \phi_{6,j+1} + \phi_{6,j-1}) = B_{7,j}$$

$i = 8, \; 3 \leq j \leq 13$

$$15\phi_{8,j} - 5(\phi_{7,j} + \phi_{8,j+1} + \phi_{8,j-1})\ \phi_{6,j} + \phi_{8,j+2} + \phi_{8,j-2} + .5(\phi_{7,j+1} + \phi_{7,j-1}) = B_{8,j}$$

$i = 1, \; j = 14$

$$14\phi_{1,14} - 10\phi_{2,14} - 5(\phi_{1,15} + \phi_{1,13}) + 2\phi_{3,14} + \phi_{2,15} + \phi_{2,13} + \phi_{1,12} = B_{1,14}$$

$i = 2,\ j = 14$

$$15\phi_{2,14} - 5(\phi_{1,14} + \phi_{3,14} + \phi_{2,15} + \phi_{2,13}) + \phi_{4,14} + \phi_{2,12} + .5(\phi_{3,15} + \phi_{3,13} + \phi_{1,15} + \phi_{1,13}) = B_{2,14}$$

$3 \leq i \leq 6,\ j = 14$

$$14\phi_{i,14} - 5(\phi_{i+1,14} + \phi_{i-1,14} + \phi_{i,15} + \phi_{i,13}) + \phi_{i+2,14} + \phi_{i-2,14} + \phi_{i,12} + .5(\phi_{i+1,15} + \phi_{i-1,15} + \phi_{i+1,13} + \phi_{i-1,13}) = B_{i,14}$$

$i = 7,\ j = 14$

$$14\phi_{7,14} - 5(\phi_{8,14} + \phi_{6,14} + \phi_{7,15} + \phi_{7,13}) + \phi_{5,14} + \phi_{7,12} + .5(\phi_{8,15} + \phi_{8,13} + \phi_{6,15} + \phi_{6,13}) = B_{7,14}$$

$i = 8,\ j = 14$

$$15\phi_{8,14} - 5(\phi_{7,14} + \phi_{8,15} + \phi_{8,13}) + \phi_{6,14} + \phi_{8,12} + .5(\phi_{7,15} + \phi_{7,13}) = B_{8,14}$$

$i = 1,\ j = 15$

$$15\phi_{1,15} - 10\phi_{2,15} - 5\phi_{1,14} + 2\phi_{3,15} + \phi_{1,13} + \phi_{2,14} = B_{1,15}$$

$i = 2,\ j = 15$

$$16\phi_{2,15} - 5(\phi_{3,15} + \phi_{1,15} + \phi_{2,14}) + \phi_{4,15} + \phi_{2,13} + .5(\phi_{3,14} + \phi_{1,14}) = B_{2,15}$$

$3 \leq i \leq 6, \; j = 15$

$$15\phi_{i,15} - 5(\phi_{i+1,15} + \phi_{i-1,15} + \phi_{i,14}) + \phi_{i+2,15} +$$
$$\phi_{i-2,15} + \phi_{i,13} + .5(\phi_{i+1,14} + \phi_{i-1,14}) = B_{i,15}$$

$i = 7, \; j = 15$

$$15\phi_{7,15} - 5(\phi_{8,15} + \phi_{6,15} + \phi_{7,14}) + \phi_{5,15} + \phi_{7,13} +$$
$$.5(\phi_{6,14} + \phi_{8,14}) = B_{7,15}$$

$i = 8, \; j = 15$

$$16\phi_{8,15} - 5(\phi_{7,15} + \phi_{8,14}) + \phi_{6,15} + \phi_{8,13} +$$
$$.5\phi_{7,14} = B_{8,15}.$$

Table 22 shows the value of all non-zero components of the constant vector.

TABLE 22

NON-ZERO COMPONENTS OF THE CONSTANT VECTOR

FOR FINITE DIFFERENCE EQUATIONS

i	j	B	i	j	B	i	j	B
1	1	-.6507132	7	5	.1031994	8	10	-.2218186
2	1	-.6482036	7	6	.0943348	8	11	-.1842433
3	1	-.6408067	7	7	.0850253	8	12	-.1496600
4	1	-.6289199	7	8	.0754938	8	13	-.1189605
5	1	-.6131988	7	9	.0659624	8	14	-.0815076
6	1	-.5945097	7	10	.0566528	8	15	-.1319692
7	1	-.4436136	7	11	.0477882	1	14	-.0123134
8	1	-1.151426	7	12	.0395879	2	14	-.0117259
1	2	.1633010	7	13	.0322536	3	14	-.0099912
2	2	.1627135	7	14	.0319480	4	14	-.0071928
3	2	.1609788	7	15	-.0093493	5	14	-.0034683
4	2	.1581804	8	3	-.4849900	6	14	.0009988
5	2	.1544560	8	4	-.4542905	1	15	.0467626
6	2	.1499888	8	5	-.4197072	2	15	.0442531
7	2	.2700273	8	6	-.3821320	3	15	.0368562
8	2	-.3714553	8	7	-.3425526	4	15	.0249694
7	3	.1187340	8	8	-.3019753	5	15	.0092483
7	4	.1113997	8	9	-.2613979	6	15	-.0094409

APPENDIX VIII

FORTRAN PROGRAMS

The three FORTRAN programs used for the solution of the discrete problem, the analytic continuum problem, and the numerical continuum problem are shown below. The letter C in the first column of the line indicates that the line is a comment statement and that it is not executable.

In the PROGRAM CRY, which solves the discrete problem, the lattice points are located by the two indices I,J. These indices are identical with the i,j indices in Figure 5.

The PROGRAM IDIS determines the solution of the analytic continuum problem. This program determines u, v, σ_x, σ_y, and τ_{xy} at points in the region $0 \leq x \leq L$, $-L \leq y \leq L$. The points at which these quantities are determined are the nodes of a rectangular grid with spacing .0625L. The nodes are identified by two indices I and J. I and J are both one at $x = 0$, $y = -L$ and I increases to the right while J increases upward.

PROGRAM NUT solves the numerical continuum problem. This program determines values of u, v, σ_x, σ_y, and τ_{xy} at nodal points of the rectangular grid shown in Figure 14. Each nodal point is located by a single index I.

I = 1 corresponds to the point i = 1, j = 1 in Figure 14. Each nodal point is then numbered in ascending order of I from left to right with the point I = 8 corresponding to i = 8, j = 1 in Figure 14. The point I = 9 in the FORTRAN program corresponds to i = 1, j = 2 in Figure 14 and then increases to I = 16 at the nodal point located by i = 8, j = 2 in Figure 14. The nodal point indicated by i = 8, j = 15 in Figure 14 is denoted by I = 120 for purposes of PROGRAM NUT.

```
      PROGRAM CRY
      PROGRAM CRY DETERMINES DISCRETE VALUES OF DISPLACEMENT
      DIMENSION U(18,33),V(18,33),DIFFV(18,33),DIFFU(18,33)
      READ 1000,U
      READ 1000,V
      PRINT 200
      PRINT 205,((I,J,(U(I,J)),(V(I,J)),J=1,33),I=1,18)
      PRINT 2
    2 FORMAT(21H   NUM              BIG)
      NUM=0
    5 DO 3 I=1,18
      DO 3 J=1,33
      DIFFU(I,J)=0.0
    3 DIFFV(I,J)=0.0
      U1=(U(2,1)+.5*(U(2,2)+V(2,2)-V(1,1)))/1.5
      DIFFU(1,1)=ABSF(U1-U(1,1))
      U(1,1)=U1
      V1=(V(1,2)+.5*(U(2,2)+V(2,2)-U(1,1)))/1.5
      DIFFV(1,1)=ABSF(V1-V(1,1))
      V(1,1)=V1
      DO 10 J=2,32
      U1=(U(2,J)+.5*(U(2,J+1)+V(2,J+1)+U(2,J-1)-V(2,J-1)))/2.
      DIFFU(1,J)=ABSF(U1-U(1,J))
      U(1,J)=U1
      V1=(V(1,J+1)+V(1,J-1)+.5*(V(2,J+1)+U(2,J+1)+V(2,J-1)
     1-U(2,J-1)))/3.
      DIFFV(1,J)=ABSF(V1-V(1,J))
   10 V(1,J)=V1
      U1=(U(2,33)+.5*(U(2,32)-V(2,32)+V(1,33)))/1.5
      DIFFU(1,33)=ABSF(U1-U(1,33))
      U(1,33)=U1
      V1=(V(1,32)+.5*(V(2,32)-U(2,32)+U(1,33)))/1.5
      DIFFV(1,33)=ABSF(V1-V(1,33))
      V(1,33)=V1
      DO 20 I=2,16
      U1=(U(I+1,33)+U(I-1,33)+.5*(U(I+1,32)-V(I+1,32)+U(I-1,32)
     1+V(I-1,32)))/3.
      DIFFU(I,33)=ABSF(U1-U(I,33))
      U(I,33)=U1
      V1=(V(I,32)+.5*(V(I+1,32)-U(I+1,32)+V(I-1,32)+U(I-1,32)))/2.
      DIFFV(I,33)=ABSF(V1-V(I,33))
   20 V(I,33)=V1
      U1=(U(16,33)+.5*(-U(17,32)-V(17,32)+U(16,32)+V(16,32)))/4.
      DIFFU(17,33)=ABSF(U1-U(17,33))
      U(17,33)=U1
      V1=(V(17,32)+.5*(V(17,32)+U(17,32)+V(16,32)+U(16,32)))/2.
      DIFFV(17,33)=ABSF(V1-V(17,33))
      V(17,33)=V1
      DO 30 K=1,14
      J=33-K
      U1=(U(16,J)+.5*(-U(17,J+1)+V(17,J+1)+U(16,J+1)-V(16,J+1)
     1+U(16,J-1)+V(16,J-1)-U(17,J-1)-V(17,J-1)))/5.
      DIFFU(17,J)=ABSF(U1-U(17,J))
      U(17,J)=U1
```

```
      V1=(1.5*(V(17,J+1)+V(17,J-1))+.5*(-U(17,J+1)+V(16,J+1)
     1-U(16,J+1)+V(16,J-1)+U(16,J-1)+U(17,J-1)))/4.
      DIFFV(17,J)=ABSF(V1-V(17,J))
   30 V(17,J)=V1
      U1=(U(16,18)+.5*(U(16,19)-V(16,19)-U(17,19)+V(17,19)
     1+U(16,17)+V(16,17)-U(17,17)-V(17,17))
     2+.4*V(17,18)-.4*V(18,17)-.13246)/5.2
      DIFFU(17,18)=ABSF(U1-U(17,18))
      U(17,18)=U1
      V1=(1.5*V(17,19)+V(17,17)+.5*(-U(16,19)+V(16,19)-U(17,19)
     1+U(16,17)+V(16,17)+U(17,17)-V(17,17))
     2+.4*U(17,18)+.8*V(18,17)+.26491)/4.8
      DIFFV(17,18)=ABSF(V1-V(17,18))
      V(17,18)=V1
      U1=(U(16,17)+.5*(-U(17,18)+V(17,18)+U(16,16)+V(16,16)
     1    +U(16,18)-V(16,18))+.05872*V(17,17)-.55872
     2    *V(18,16)-.68507)/3.77936
      DIFFU(17,17)=ABSF(U1-U(17,17))
      U(17,17)=U1
      V1=(1.5*V(17,18)+V(17,16)+.5*(-U(17,18)+U(16,16)+V(16,16)
     1    -U(16,18)+V(16,18))-.15080*U(17,17)+.69841*V(18,16)
     2     +.23127)/4.19841
      DIFFV(17,17)=ABSF(V1-V(17,17))
      V(17,17)=V1
      DO 40 K=17,31
      J=33-K
      U1=(U(16,J)+.5*(U(16,J+1)-V(16,J+1)+U(16,J-1))
     1  -.63246*(V(18,J-1)-V(18,J+1))-.91886)/3.63246
      DIFFU(17,J)=ABSF(U1-U(17,J))
      U(17,J)=U1
      V1=(V(17,J+1)+V(17,J-1)+.5*(U(16,J-1)+V(16,J-1)-U(16,J+1)
     1  +V(16,J+1))+.63246*(V(18,J-1)+V(18,J+1)))/4.26492
      DIFFV(17,J)=ABSF(V1-V(17,J))
   40 V(17,J)=V1
      U1=(U(16,1)+.5*(U(16,2)-V(16,2)+V(17,1))+.63246
     1    *(V(18,2)-V(17,1))-.70943)/2.81623
      DIFFU(17,1)=ABSF(U1-U(17,1))
      U(17,1)=U1
      V1=(V(17,2)+.5*(-U(16,2)+V(16,2))+.18377*U(17,1)
     1    +.63246*V(18,2)-.20943)/2.13246
      DIFFV(17,1)=ABSF(V1-V(17,1))
      V(17,1)=V1
      DO 50 J=2,15
      V1=(V(18,J+1)+V(18,J-1)-.63246*(U(17,J+1)-U(17,J-1))
     1  +1.26492*(V(17,J+1)+V(17,J-1)))/4.52984
      DIFFV(J)=ABSF(V1-V(18,J))
   50 V(18,J)=V1
      V1=(V(18,17)+V(18,15)+.63246*U(17,15)+1.26492*V(17,15)
     1    -.69841*U(17,17)+1.39682*V(17,17)-.04170)/4.66174
      DIFFV(18,16)=ABSF(V1-V(18,16))
      V(18,16)=V1
      V1=(V(18,16)+.63246*U(17,16)+1.26492*V(17,16)-.8*U(17,18)
     1    +1.6*V(17,18)+.19764)/3.86492
      DIFFV(18,17)=ABSF(V1-V(18,17))
```

```
      V(18,17)=V1
      DO 60 K=1,15
      I=17-K
      U1=(U(I+1,1)+U(I-1,1)+.5*(U(I+1,2)+V(I+1,2)+U(I-1,2)-V(I-1,2)))/3.
      DIFFU(I,1)=ABSF(U1-U(I,1))
      U(I,1)=U1
      V1=(V(I,2)+.5*(U(I+1,2)+V(I+1,2)-U(I-1,2)+V(I-1,2)))/2.
      DIFFV(I,1)=ABSF(V1-V(I,1))
   60 V(I,1)=V1
      DO 70 I=2,16
      DO 70 J=2,32
      U1=(U(I+1,J)+U(I-1,J)+.5*(U(I+1,J+1)+V(I+1,J+1)+U(I-1,J+1)
     1-V(I-1,J+1)+U(I-1,J-1)+V(I-1,J-1)+U(I+1,J-1)-V(I+1,J-1)))/4.
      DIFFU(I,J)=ABSF(U1-U(I,J))
      U(I,J)=U1
      V1=(V(I,J+1)+V(I,J-1)+.5*(V(I+1,J+1)+U(I+1,J+1)+V(I-1,J+1)
     1-U(I-1,J+1)+V(I-1,J-1)+U(I-1,J-1)+V(I+1,J-1)-U(I+1,J-1)))/4.
      DIFFV(I,J)=ABSF(V1-V(I,J))
   70 V(I,J)=V1
      NUM=NUM+1
      IF(NUM-5800)160,160,500
  500 BIGU=0.0
      DO 90 I=1,18
      DO 90 J=1,33
      IF(BIGU-DIFFU(I,J))80,90,90
   80 BIGU=DIFFU(I,J)
   90 CONTINUE
      BIGV=0.0
      DO 120 I=1,18
      DO 120 J=1,33
      IF(BIGV-DIFFV(I,J))110,120,120
  110 BIGV=DIFFV(I,J)
  120 CONTINUE
      IF(BIGV-BIGU)130,130,140
  130 BIG=BIGU
      GO TO 144
  140 BIG=BIGV
  144 PRINT 145,NUM,BIG
  145 FORMAT(I6,E15.6)
  160 IF(NUM-6000)5,150,150
  150 PRINT 195
  195 FORMAT(22H DISPLACEMENT SOLUTION)
      PRINT 200
  200 FORMAT(40H      I     J                  U                 V)
      PRINT 205,((I,J,(U(I,J)),(V(I,J)),J=1,33),I=1,18)
  205 FORMAT(2I5,2E15.6)
  300 FORMAT(3E15.6)
      PRINT 205,((I,J,(DIFFU(I,J)),(DIFFV(I,J)),J=1,33)
     1     ,I=1,18)
      PUNCH 1000, U
      PUNCH 1000, V
 1000 FORMAT(3E20.6)
      K=5
 1500 CALL DXST(K,U,V)
```

```
      IF(K-13)2000,2001,2001
 2000 K=K+4
      GO TO 1500
 2001 CONTINUE
      END
      SUBROUTINE DXST(K,U,V)
C     SUBROUTINE DXST DETERMINES THE LATTICE FORCES ACROSS
C     A VERTICAL PLANE
      DIMENSION U(18,33),V(18,33),FX(33),FY(33)
      KK=K-1
      FX(1)=1.5*U(K,1)-U(KK,1)-.5*(U(KK,2)+V(K,1)-V(KK,2))
      FY(1)=.5*(U(K,1)-U(KK,2)-V(K,1)+V(KK,2))
      DO 20 J=2,32
      FX(J)=2.*U(K,J)-U(KK,J)-.5*(U(KK,J+1)
     1   -V(KK,J+1)+U(KK,J-1)+V(KK,J-1))
   20 FY(J)=-V(K,J)-.5*(U(KK,J+1)-V(KK,J+1)-U(KK,J-1)-V(KK,J-1))
      FX(33)=1.5*U(K,33)-U(KK,33)-.5*(U(KK,33)
     1   -V(K,33)+V(KK,32))
      FY(33)=-.5*(U(K,33)-U(KK,32)+V(K,33)-V(KK,32))
      SUMX=0.0
      SUMY=0.0
      DO 25 J=1,33
      SUMX=SUMX+FX(J)
   25 SUMY=SUMY+FY(J)
      PRINT 30,K
   30 FORMAT(5H K = I2)
      PRINT 40
   40 FORMAT(44H    J                    FX                    FY)
      PRINT 50,(J,(FX(J)),(FY(J)),J=1,33)
   50 FORMAT(I4,2E20.6)
      PRINT 60,SUMX
   60 FORMAT(8H SUMX = E20.6)
      PRINT 70,SUMY
   70 FORMAT(8H SUMY = E20.6)
      END
```

```
      PROGRAM IDIS
C     PROGRAM IDIS DETERMINES ANALYTIC VALUES OF
C     STRESS AND DISPLACEMENT
      DIMENSION Y(33),X(17),XP(17,17),S1(33,17),S2(33,17),
     1 X2P(17,17),U(33,17),V(33,17),R1(33,17),R2(33,17)
     2      ,SX(33,17),SY(33,17),SXY(33,17)
C THIS PROGRAM GIVES DISPLACEMENTS FOR THE ANALYTIC SOLUTION
      Z=.3208
      E1=ATANF(Z)
      E2=ATANF(-Z)
      T=0.0
      Y(1)=-1.0
      X(1)=0.0
      DO 10 J=2,33
   10 Y(J)=Y(J-1)+.0625
      DO 15 I=2,17
   15 X(I)=X(I-1)+.0625
      DO 20 J=18,33
      DO 20 I=1,17
   20 S1(J,I)=ATANF((.790569*Y(J))/(X(I)+.612372*Y(J)))
     1      +6.283185
      DO 25 I=2,17
   25 S1(17,I)=6.283185
      DO 30 J=1,16
      DO 30 I=1,17
      XP(J,I)=X(I)+.612372*Y(J)
      IF(XP(J,I)-T)31,32,33
   31 S1(J,I)=ATANF((.790569*Y(J))/(XP(J,I)))+3.141593
      GO TO 30
   32 S1(J,I)=1.5*3.141593
      GO TO 30
   33 S1(J,I)=ATANF((.790569*Y(J))/(X(I)+.612372*Y(J)))
     1      +6.283185
   30 CONTINUE
C THE DO LOOPS 20,25,AND 30 GIVE ALL IMAGINARY VALUES OF LN Z(1)
      DO 40 J=1,16
      DO 40 I=1,17
   40 S2(J,I)=ATANF((-.790569*Y(J))/(X(I)-.612372*Y(J)))
      DO 45 I=2,17
   45 S2(17,I)=0.0
      DO 50 J=18,33
      DO 50 I=1,17
      X2P(J,I)=X(I)-.612372*Y(J)
      IF(X2P(J,I)-T)51,52,53
   51 S2(J,I)=ATANF((-.790569*Y(J))/(X2P(J,I)))-3.141593
      GO TO 50
   52 S2(J,I)=-3.141593/2.
      GO TO 50
   53 S2(J,I)=ATANF((-.790569*Y(J))/(X2P(J,I)))
   50 CONTINUE
C THE DO LOOPS 40,45,AND 50 GIVE THE IMAGINARY PARTS OF LN Z(2)
C THE VALUES OF S1(17,1)AND S2(17,1)ARE INFINITY, THEREFORE ASSIGN
C ARBITRARILY LARGE VALUES TO THEM
      S1(17,1)=10.**6
```

```
      S2(17,1)=10.**6
C THE DO LOOPS 60 AND 65 GIVE THE REAL PARTS OF LN Z(1) AND LN Z(2)
      DO 60 J=1,33
      DO 60 I=2,17
      R1(J,I)=.5*LOGF(X(I)**2+Y(J)**2+2.*.612372*X(I)*Y(J))
   60 R2(J,I)=.5*LOGF(X(I)**2+Y(J)**2-2.*.612372*X(I)*Y(J))
      DO 65 J=1,16
      R1(J,1)=.5*LOGF(Y(J)**2)
   65 R2(J,1)=.5*LOGF(Y(J)**2)
      DO 66 J=18,33
      R1(J,1)=.5*LOGF(Y(J)**2)
   66 R2(J,1)=.5*LOGF(Y(J)**2)
C THE REAL PARTS OF LN Z(1) AND LN Z(I) ARE UNDEFINED AT THE POINT
C (17,1)THEREFORE GIVE THEM ARBITRARILY LARGE VALUES THERE
      R1(17,1)=10.**12
      R2(17,1)=10.**12
C THE DO LOOP 70 GIVES THE DISPLACEMENTS FOR THE ANALYTIC SOLUTION
      DO 70 J=1,33
      DO 70 I=1,17
      U(J,I)=(((-.75)/.968246)*(R1(J,I)-R2(J,I))-(S1(J,I)
     1      -S2(J,I))+3.*3.141593)/(4.*3.141593)
   70 V(J,I)=(.316227*(R1(J,I)+R2(J,I))+1.224744*(S1(J,I)
     1   +S2(J,I)-2.*.911738-3.141593))/(4.*3.141593)
      PRINT 75 ,E1,E2
   75 FORMAT(2E15.6)
      PRINT 95
   95 FORMAT(//63H   J   I            X             Y                S1
     1       S2)
      PRINT 100,((J,I,(X(I)),(Y(J)),(S1(J,I)),(S2(J,I)),I=1,17)
     1  ,J=1,33)
      PRINT 96
   96 FORMAT(//65H    J    I            X             Y              R1
     1          R2)
      PRINT 100,((J,I,(X(I)),(Y(J)),(R1(J,I)),(R2(J,I)),I=1,17)
     1  ,J=1,33)
      PRINT 85
   85 FORMAT(//36H DISPLACEMENTS FOR ANALYTIC SOLUTION)
      PRINT 80
   80 FORMAT(//62H   J   I            X             Y                U
     1       V)
      PRINT 100,((J,I,(X(I)),(Y(J)),(U(J,I)),(V(J,I)),
     1  I=1,17),J=1,33)
  100 FORMAT(2I4,2E12.4,2E15.6)
      SX(17,1)=10.**12
      SY(17,1)=10.**12
      SXY(17,1)=10.**12
      L1=1
      L2=16
  113 DO 110 J=L1,L2
      DO 110 I=1,17
      SX(J,I)=Y(J)*(.11324073*X(I)**2+.07549382*Y(J)**2)
     1    /(X(I)**4+.5*X(I)**2*Y(J)**2+Y(J)**4)
      SY(J,I)=.07549382*Y(J)*(Y(J)**2-X(I)**2)/(X(I)**4
     1    +.5*X(I)**2*Y(J)**2+Y(J)**4)
```

```
110 SXY(J,I)=.07549382*X(I)*(Y(J)**2-X(I)**2)/(X(I)**4
   1     +.5*X(I)**2*Y(J)**2+Y(J)**4)
    IF(L2-33)111,112,112
111 L1=17
    L2=33
    GO TO 113
112 DO 120 I=2,17
    SX(17,I)=0.0
    SY(17,I)=0.0
120 SXY(17,I)=-.07549382/X(I)
    PRINT 130
130 FORMAT(68H     J    I                       SX                        SY
   1            SXY)
    PRINT 140,((J,I,(SX(J,I)),(SY(J,I)),(SXY(J,I)),I=1,17)
   1      ,J=1,33)
140 FORMAT(2I5,3E20.6)
    END
```

```
      PROGRAM NUT
C     PROGRAM NUT DETERMINES THE STRESS FUNCTION, STRESSES,
C     AND DISPLACEMENTS FOR THE NUMERICAL SOLUTION
      DIMENSION BFEE(17),SFEE(31),UFEE(17),BBFEE(17),
     1   SSFEE(31),UUFEE(17),B(496),X(496),TBXY(17),TSXY(31),TUXY(17)
     2   ,DBFEE(17),DSFEE(31),DUFEE(17)
      READ 1,N,N2,DEL
    1 FORMAT(2I4,F6.4)
      N1=(N-1)*N2
      CALL FCAL(DEL,N,N2,BFEE,DBFEE,SFEE,
     1     DSFEE,UFEE,DUFEE,DBS,DUS)
      CALL BCAL(N,N2,BFEE,SFEE,UFEE,DBFEE,
     1     DSFEE,DUFEE,B,DEL)
      READ 400,X
  400 FORMAT(4E17.8)
      CALL SFIT(N,N2,B,X,SUS,SBS,DUS,DBS,
     1   BFEE,BBFEE,DBFEE,SFEE,SSFEE,DSFEE,
     2   UFEE,UUFEE,DUFEE,DEL)
      CALL STRESS( N,N2,DEL,X,BFEE,BBFEE,SFEE,SSFEE,
     1   UFEE,UUFEE,TBXY,TSXY,TUXY,SUS,SBS)
      CALL DISP(DEL,N,N2,X,BFEE,BBFEE,SFEE,SSFEE,
     1   UFEE,UUFEE)
      PUNCH 400,(X(I),I=1,N1)
      END
      SUBROUTINE FCAL(DEL,N,N2,BFEE,DBFEE,SFEE,DSFEE,
C     SUBROUTINE FCAL DETERMINES BOUNDARY VALUES OF THE
C     STRESS FUNCTION AND ITS DERIVATIVES
     1   UFEE,DUFEE,DBS,DUS)
      DIMENSION Z1(17),Z2(31),BFEE(17),DBFEE(17),UFEE(17),
     1   DUFEE(17),SFEE(31),DSFEE(31),SIGX(31),PSIGX(31),
     2   SIGY(17),PSIGY(17),B(50)
      Z1(1)=0.0
      DO 11 J=2,N
   11 Z1(J)=Z1(J-1)+DEL
      Z2(1)=-1.0+DEL
      DO 6 J=2,N2
    6 Z2(J)=Z2(J-1)+DEL
      H=SQRTF(.9375)
      G=.5*ACOSF(-.25)
      P=6.2831853
      SG=SINF(G)
      CG=COSF(G)
      D=2.-4.*(CG**2)
      C1=-(((-.750/H)*.5625+.25*H)*CG+((-.750*.25)-.5625)*SG)/P
      C2=(((-.750/H)*.5625+.25*H)*CG-((-.750*.25)-.5625)*SG)/P
      DO 13 J=1,N
   13 SIGY(J)=C2*(Z1(J)**2-1.)/(Z1(J)**4+D*Z1(J)**2+1.)
      DO 900 J=1,N2
  900 SIGX(J)=(-C1*Z2(J)-C2*Z2(J)**3)/(Z2(J)**4+D*Z2(J)**2+1.)
      DD=SQRTF(4.-D**2)
      DO 5 J=1,N
      UFEE(J)=(.25*C2/CG)*Z1(J)*LOGF((Z1(J)**2-2.*CG*Z1(J)+1.)/
     1  (Z1(J)**2+2.*CG*Z1(J)+1.))-.25*C2*LOGF(Z1(J)**4+D*Z1(J)**2+1.)
     2  +(C2*(1.+.5*D)/DD)*ATANF((2.*Z1(J)**2+D)/DD)
```

```
      BFEE(J)=-UFEE(J)+((C2+D*C2-C1)/(4.*CG))*LOGF((1.-CG)/(1.+CG))
     1   +((C2+C2*D-C1)/(4.*SG))*(P/2.)-2.*C2
      DUFEE(J)=((C2*(1.+.5*D)/DD)*ATANF((2.*Z1(J)**2+D)/DD)
     1   -.25*C2*LOGF(Z1(J)**4+D*Z1(J)**2+1.))
    5 DBFEE(J)=DUFEE(J)
      DO 7 J=1,N2
      SFEE(J)=((-C1+.5*D*C2)/DD)*Z2(J)*ATANF((2.*Z2(J)**2+D)/DD)
     1   -.25*C2*Z2(J)*LOGF(Z2(J)**4+D*Z2(J)**2+1.)+((D*C2-C1-C2)
     2   /(8.*CG))*LOGF((Z2(J)**2+2.*CG*Z2(J)+1.)/(Z2(J)**2
     3   -2.*CG*Z2(J)+1.))-((C2+C2*D-C1)/(4.*SG))*ATANF((2.*SG*Z2(J))
     4   /(1.-Z2(J)**2))+C2*Z2(J)+(((C1+C2)/DD)*ATANF((2.+D)/DD))*Z2(J)
     5   +((C2+D*C2-C1)/(8.*CG))*LOGF((1.-CG)/(1.+CG))
     6   +(C2+C2*D-C1)*P/(16.*SG)-C2
    7 DSFEE(J)=((.25*C2/CG)*LOGF((Z2(J)**2-2.*CG*Z2(J)+1.)
     1   /(Z2(J)**2+2.*CG*Z2(J)+1.)))
      DBS=(.25*C2/CG)*LOGF((1.+CG)/(1.-CG))
      DUS=(.25*C2/CG)*LOGF((1.+CG)/(1.-CG))
      PSIGY(1)=2.*(UFEE(2)-UFEE(1))/DEL**2
      M4=N-1
      DO 8 J=2,M4
    8 PSIGY(J)=(UFEE(J-1)-2.*UFEE(J)+UFEE(J+1))/DEL**2
      PSIGX(1)=(SFEE(2)-2.*SFEE(1)+BFEE(N))/DEL**2
      N3=N2-1
      DO 9 J=2,N3
    9 PSIGX(J)=(SFEE(J-1)-2.*SFEE(J)+SFEE(J+1))/DEL**2
      PSIGX(N2)=(UFEE(N)-2.*SFEE(N2)+SFEE(N3))/DEL**2
      PRINT 12
   12 FORMAT(/43H                    EXACT STRESS    APPROX STRESS)
      PRINT 14,(J,(Z1(J)),(SIGY(J)),(PSIGY(J )),J=1,M4)
   14 FORMAT(I4,E15.4,2E20.8)
      PRINT 14,(J,(Z2(J)),(SIGX(J)),(PSIGX(J)),J=1,N2)
      PRINT 21
   21 FORMAT(47H BOUNDARY VALUES OF S. F. AND NORMAL DERIVATIVES)
      PRINT 22,(J,(Z1(J)),(BFEE(J)),(DBFEE(J)),
     1   (UFEE(J)),(DUFEE(J)),J=1,N)
   22 FORMAT(I3,E8.5,4E15.6)
      PRINT 23,(J,(Z2(J)),(SFEE(J)),(DSFEE(J)),J=1,N2)
   23 FORMAT(I3,E15.4,2E15.6)
      END
      SUBROUTINE BCAL(N,N2,BFEE,SFEE,UFEE,DBFEE,
     1   DSFEE,DUFEE,B,DEL)
C     SUBROUTINE BCAL DETERMINES THE CONSTANT VECTOR FOR
C     THE SYSTEM OF FINITE DIFFERENCE COMPATIBILITY EQUATIONS
      DIMENSION BFEE(17),DBFEE(17),SFEE(31),DSFEE(31),
     1   UFEE(17),DUFEE(17),B(496)
      N1=(N-1)*N2
      DO 10 I=1,N1
   10 B(I)=0.0
      B(1)=5.*BFEE(1)-BFEE(2)+2.*DEL*DBFEE(1)
      M=N-2
      DO 20 J=2,M
   20 B(J)=5.*BFEE(J)-.5*BFEE(J+1)-.5*BFEE(J-1)
     1   +2.*DEL*DBFEE(J)
      B(M)=B(M)-SFEE(1)
```

```
      M4=N-1
      B(M4)=5.*BFEE(M4)+5.*SFEE(1)-.5*BFEE(M)-.5*BFEE(N)
     1    -.5*SFEE(2)+2.*DEL*(DBFEE(M4)-DSFEE(1))
      M1=2*N-3
      DO 30 J=N,M1
   30 B(J)=-BFEE(J-M4)
      B(M1)=B(M1)-SFEE(2)
      M2=M1+1
      M3=(N-1)*(N2-1)
      DO 40 J=M2,M3,M4
      K=J/M4
   40 B(J)=5.*SFEE(K)-.5*SFEE(K-1)-.5*SFEE(K+1)
     1    -2.*DEL*DSFEE(K)
      B(M2)=B(M2)-BFEE(M4)
      B(M3)=B(M3)-UFEE(M4)
      L5=(N-1)*(N2-1)+1
      B(L5)=5.*UFEE(1)-UFEE(2)-2.*DEL*DUFEE(1)
      DO 50 J=2,M
   50 B(J+M3)=5.*UFEE(J)-.5*UFEE(J-1)-.5*UFEE(J+1)
     1        -2.*DEL*DUFEE(J)
      L11=(N-1)*N2-1
      L12=L11+1
      L13=N2-1
      B(L11)=B(L11)-SFEE(N2)
      B(L12)=5.*UFEE(M4)+5.*SFEE(N2)-.5*UFEE(M)-.5*UFEE(N)
     1    -.5*SFEE(L13)-2.*DEL*(DSFEE(N2)+DUFEE(M4))
      N3=3*M4-1
      N4=M4*(N2-2)-1
      DO 51 I=N3,N4,M4
      J=(I+1)/M4
   51 B(I)=-SFEE(J)
      N5=M4*(N2-2)
      DO 52 J=1,M
   52 B(J+N5)=-UFEE(J)
      N6=M3-1
      B(N6)=B(N6)-SFEE(L13)
      PRINT 55
   55 FORMAT(/9H B VALUES)
      PRINT 60,(I,(B(I)),I=1,N1)
   60 FORMAT(4(I8,E13.6))
      END
      SUBROUTINE SFIT(N,N2,B,X,SUS,SBS,DUS,DBS,
     1    BFEE,BBFEE,DBFEE,SFEE,SSFEE,DSFEE,UFEE,
     2    UUFEE,DUFEE,DEL)
C     SUBROUTINE SFIT ITERATES TO FIND THE STRESS FUNCTION
C     VECTOR
      DIMENSION X(496),X1(496),DIFF(496),B(496),
     1    BFEE(17),BBFEE(17),DBFEE(17),SFEE(31),SSFEE(31),
     2  DSFEE(31),UFEE(17),UUFEE(17),DUFEE(17)
      N1=N2*(N-1)
      M4=N-1
      M=N-2
      L11=(N-1)*N2-1
      M3=(N-1)*(N2-1)
```

```
      L5=(N-1)*(N2-1)+1
      LL2=N1-3*M4+3
      M6=2*M4
      NUM=0
      PRINT 70
   70 FORMAT(/13H NUM       BIG)
   80 DO 71 I=1,N1
   71 DIFF(I)=0.0
      L=2*M4+3
  120 LL=L+M4-5
      DO 90 I=L,LL
      X1(I)=(5.*(X(I+1)+X(I-1)+X(I+M4)+X(I-M4))-X(I+2)-X(I-2)
     1-X(I+M6)-X(I-M6)-.5*(X(I+N)+X(I-N)+X(I-M)+X(I+M)))/14.
      DIFF(I)=ABSF(X1(I)-X(I))
   90 X(I)=X1(I)
      IF(L-LL2)100,110,110
  100 L=L+M4
      GO TO 120
  110 LL3=2*M4+1
      LL4=LL2-2
      DO 130 I=LL3,LL4,M4
      X1(I)=(B(I)+10.*X(I+1)+5.*X(I+M4)+5.*X(I-M4)-X(I+M6)-X(I-M6)
     1-2.*X(I+2)-X(I+N)-X(I-M))/14.
      DIFF(I)=ABSF(X1(I)-X(I))
  130 X(I)=X1(I)
      LL5=LL3+1
      LL6=LL4+1
      DO 140 I=LL5,LL6,M4
      X1(I)=(B(I)+5.*(X(I+1)+X(I-1)+X(I+M4)+X(I-M4))-X(I+M6)-X(I-M6)
     1-X(I+2)-.5*(X(I+N)+X(I-N)+X(I+M)+X(I-M)))/15.
      DIFF(I)=ABSF(X1(I)-X(I))
  140 X(I)=X1(I)
      LL7=3*M4-1
      LL8=M4*(N2-2)-1
      DO 150 I=LL7,LL8,M4
      X1(I)=(B(I)+5.*(X(I+1)+X(I-1)+X(I+M4)+X(I-M4))-X(I-2)-X(I+M6)-
     1X(I-M6)-.5*(X(I+N)+X(I-N)+X(I+M)+X(I-M)))/14.
      DIFF(I)=ABSF(X1(I)-X(I))
  150 X(I)=X1(I)
      LL9=LL7+1
      LL10=LL8+1
      DO 160 I=LL9,LL10,M4
      X1(I)=(B(I)+5.*(X(I-1)+X(I+M4)+X(I-M4))-X(I-2)-X(I+M6)-X(I-M6)
     1     -.5*X(I+M)-.5*X(I-N))/15.
      DIFF(I)=ABSF(X1(I)-X(I))
  160 X(I)=X1(I)
      L1=M4+3
      LL1=M6-2
      DO 165 I=L1,LL1
      X1(I)=(B(I)+5.*(X(I+1)+X(I-1)+X(I+M4)+X(I-M4))-X(I+2)-X(I-2)
     1-X(I+M6)-.5*(X(I+N)+X(I-N)+X(I+M)+X(I-M)))/14.
      DIFF(I)=ABSF(X1(I)-X(I))
  165 X(I)=X1(I)
      L2=M4-2
```

```
      DO 170 I=3,L2
      X1(I)=(B(I)+5.*(X(I+1)+X(I-1)+X(I+M4))-X(I+2)-X(I-2)-X(I+M6)
     1      -.5*(X(I+N)+X(I+M)))/15.
      DIFF(I)=ABSF(X1(I)-X(I))
  170 X(I)=X1(I)
      NN1=M4*(N2-2)+3
      NN2=M4*(N2-1)-2
      DO 175 I=NN1,NN2
      X1(I)=(B(I)+5.*(X(I+1)+X(I-1)+X(I+M4)+X(I-M4))-X(I-M6)-X(I-2)
     1-X(I+2)-.5*(X(I+N)+X(I-N)+X(I+M)+X(I-M)))/14.
      DIFF(I)=ABSF(X1(I)-X(I))
  175 X(I)=X1(I)
      NN3=NN1+M4
      NN4=NN2+M4
      DO 180 I=NN3,NN4
      X1(I)=(B(I)+5.*(X(I+1)+X(I-1)+X(I-M4))-X(I+2)-X(I-2)-X(I-M6)
     1      -.5*(X(I-N)+X(I-M)))/15.
      DIFF(I)=ABSF(X1(I)-X(I))
  180 X(I)=X1(I)
      NN5=N+1
      NN6=2*N-1
      NN7=3*N-2
      NN8=2*N
      NN9=N+2
      NM1=N+3
      NM2=2*N+1
      NM3=3*N-1
      X1(1)=(B(1)+10.*X(2)+5.*X(N)-2.*X(3)
     1    -X(NN5)-X(NN6))/15.
      DIFF(1)=ABSF(X1(1)-X(1))
      X(1)=X1(1)
      X1(2)=(B(2)+5.*(X(1)+X(3)+X(NN5))-X(4)-X(NN8)-.5*
     1       (X(N)+X(NN9)))/16.
      DIFF(2)=ABSF(X1(2)-X(2))
      X(2)=X1(2)
      X1(N)=(B(N)+10.*X(NN5)+5.*(X(NN6)+X(1))-X(NN7)-2.*X(NN9)
     1-X(NN8)-X(2))/14.
      DIFF(N)=ABSF(X1(N)-X(N))
      X(N)=X1(N)
      X1(NN5)=(B(NN5)+5.*(X(NN9)+X(N)+X(2)+X(NN8))-X(NM3)-X(NM1)
     1-.5*(X(1)+X(3)+X(NN6)+X(NM2)))/15.
      DIFF(NN5)=ABSF(X1(NN5)-X(NN5))
      X(NN5)=X1(NN5)
      NM4=3*M4
      NM5=4*M4
      NM6=3*M4-1
      NM7=M6-1
      NM8=M6-2
      NM9=N-3
      NL=4*M4-1
      NL1=3*M4-2
      NL2=M6-3
      NL3=N-4
      X1(M4)=(B(M4)+5.*(X(M6)+X(M))-X(NM4)-X(NM9)
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```
1     -.5*X(NM7))/16.
      DIFF(M4)=ABSF(X1(M4)-X(M4))
      X(M4)=X1(M4)
      X1(M)=(B(M)+5.*(X(M4)+X(NM7)+X(NM9))-X(NM6)-X(NL3)-.5*(X(M6)
1      +X(NM8)))/15.
      DIFF(M)=ABSF(X1(M)-X(M))
      X(M)=X1(M)
      X1(M6)=(B(M6)+5.*(X(NM4)+X(M4)+X(NM7))-X(NM5)-X(NM8)-.5*(X(NM6)
1     +X(M)))/15.
      DIFF(M6)=ABSF(X1(M6)-X(M6))
      X(M6)=X1(M6)
      X1(NM7)=(B(NM7)+5.*(X(NM6)+X(M6)+X(NM8)+X(M))-X(NL)-X(NL2)
1-.5*(X(NM4)+X(M4)+X(NL1)+X(NM9)))/14.
      DIFF(NM7)=ABSF(X1(NM7)-X(NM7))
      X(NM7)=X1(NM7)
      NL4=M4*(N2-3)
      NL5=M4*(N2-3)-1
      NL6=M4*(N2-2)-2
      NL7=M4*(N2-1)-1
      NL8=M4*N2-2
      NL9=M4*N2-3
      NJ=M4*(N2-1)-3
      X1(N1)=(B(N1)+5.*(X(L11)+X(M3))-X(NL8)-X(LL10)
1     -.5*X(NL7))/16.
      DIFF(N1)=ABSF(X1(N1)-X(N1))
      X(N1)=X1(N1)
      X1(M3)=(B(M3)+5.*(X(N1)+X(NL7)+X(LL10))-X(NN2)-X(NL4)
1     -.5*(X(L11)+X(LL8)))/15.
      DIFF(M3)=ABSF(X1(M3)-X(M3))
      X(M3)=X1(M3)
      X1(L11)=(B(L11)+5.*(X(NL8)+X(NL7)+X(N1))-X(NL9)-X(LL8)-
1      .5*(X(NN2)+X(M3)))/15.
      DIFF(L11)=ABSF(X1(L11)-X(L11))
      X(L11)=X1(L11)
      X1(NL7)=(B(NL7)+5.*(X(L11)+X(NN2)+X(M3)+X(LL8))-X(NJ)
1-X(NL5)-.5*(X(LL10)+X(N1)+X(NL8)+X(NL6)))/14.
      DIFF(NL7)=ABSF(X1(NL7)-X(NL7))
      X(NL7)=X1(NL7)
      NJ1=M4*(N2-1)+2
      NJ2=NJ1+2
      NJ3=M4*(N2-2)+1
      NJ4=NJ3+1
      NJ5=NJ3+3
      NJ6=M4*(N2-3)+1
      NJ7=NJ6+1
      NJ8=NJ6+2
      NJ9=M4*(N2-4)+1
      NK=NJ9+1
      X1(L5)=(B(L5)+10.*X(NJ1)+5.*X(NJ3)-2.*X(NN3)
1      -X(NJ6)-X(NJ4))/15.
      DIFF(L5)=ABSF(X1(L5)-X(L5))
      X(L5)=X1(L5)
      X1(NJ1)=(B(NJ1)+5.*(X(NN3)+X(NJ4)+X(L5))-X(NJ2)-X(NJ7)
1     -.5*(X(NN1)+X(NJ3)))/16.
```

```
      DIFF(NJ1)=ABSF(X1(NJ1)-X(NJ1))
      X(NJ1)=X1(NJ1)
      X1(NJ3)=(B(NJ3)+10.*X(NJ4)+5.*(X(L5)+X(NJ6))-X(NJ9)
     1-2.*X(NN1)-X(NJ1)-X(NJ7))/14.
      DIFF(NJ3)=ABSF(X1(NJ3)-X(NJ3))
      X(NJ3)=X1(NJ3)
      X1(NJ4)=(B(NJ4)+5.*(X(NJ1)+X(NN1)+X(NJ7)+X(NJ3))-X(NJ5)-X(NK)
     1-.5*(X(L5)+X(NN3)+X(NJ6)+X(NJ8)))/15.
      DIFF(NJ4)=ABSF(X1(NJ4)-X(NJ4))
      X(NJ4)=X1(NJ4)
      NUM=NUM+1
      IF(NUM-8000)80,302,302
  302 BIG=0.0
      DO 300 I=1,N1
      IF(BIG-DIFF(I))301,300,300
  301 BIG=DIFF(I)
  300 CONTINUE
  600 PRINT188,NUM,BIG
  188 FORMAT(I5,E15.6)
  189 PRINT  194
  194 FORMAT(23H STRESS FUNCTION VALUES)
      PRINT 195,(I,(X(I)),I=1,N1)
  195 FORMAT(/4(I8,E15.6))
      DO 1000 I=1,M4
      J=M3+I
      BBFEE(I)=X(I)-2.*DEL*DBFEE(I)
 1000 UUFEE(I)=X(J)+2.*DEL*DUFEE(I)
      DO 1100 I=1,N2
      J=M4*I
 1100 SSFEE(I)=X(J)+2.*DEL*DSFEE(I)
      BBFEE(N)=SFEE(1)-2.*DEL*DBFEE(N)
      UUFEE(N)=SFEE(N2)+2.*DEL*DUFEE(N)
      SUS=UFEE(M4)+2.*DEL*DUS
      SBS=BFEE(M4)+2.*DEL*DBS
      PRINT 1099
 1099 FORMAT(31H EXTRA BOUNDARY VALUES OF S. F.)
      PRINT 1101,(I,(UUFEE(I)),(BBFEE(I)),I=1,N)
 1101 FORMAT(I4,2E20.8)
      PRINT 1102,(I,(SSFEE(I)),I=1,N2)
 1102 FORMAT(I4,E20.8)
      PRINT 1103,SUS
 1103 FORMAT(7H SUS = E20.8)
      PRINT 1104,SBS
 1104 FORMAT(7H SBS = E20.8)
      END
      SUBROUTINE STRESS(N,N2,DEL,X,BFEE,BBFEE,SFEE,SSFEE,
     1   UFEE,UUFEE,TBXY,TSXY,TUXY,SUS,SBS)
C     SUBROUTINE STRESS DETERMINES INTERIOR AND BOUNDARY
C     VALUES OF STRESS
      DIMENSION X(496),SBXY(17),SSXY(31),SUXY(17),TBXY(17),
     1   TSXY(31),TUXY(17),SX(496),SY(496),SXY(496),BFEE(17),
     2   BBFEE(17),SFEE(31),SSFEE(31),UFEE(17),UUFEE(17)
     3    ,Z1(17),Z2(31),BSX(17),SSY(31)
      M=N-2
```

```
      M1=(N-1)*(N2-1)-1
      M2=(N-1)*(N2-1)+1
      M4=N-1
      Z1(1)=0.0
      DO 1 I=2,M4
    1 Z1(I)=Z1(I-1)+DEL
      Z2(1)=-1.+DEL
      DO 2 I=2,N2
    2 Z2(I)=Z2(I-1)+DEL
      DO3 I=1,M4
      TBXY(I)=.075493818*(Z1(I)**3-Z1(I))/(Z1(I)**4
     1     +.5*Z1(I)**2+1.)
    3 TUXY(I)=TBXY(I)
      DO 4 I=1,N2
    4 TSXY(I)=.075493818*(1.-Z2(I)**2)
     1     /(Z2(I)**4+.5*Z2(I)**2+1.)
      SBXY(1)=0.0
      SUXY(1)=0.0
      DO 5 I=2,M
      SBXY(I)=-(X(I+1)-X(I-1)-BBFEE(I+1)+BBFEE(I-1))/(4.*DEL**2)
    5 SUXY(I)=-(X(I+M1)-X(I+M2)-UUFEE(I-1)+UUFEE(I+1))/(4.*DEL**2)
      SBXY(M4)=-(SFEE(1)-BBFEE(N)-X(M)+BBFEE(M))/(4.*DEL**2)
      M3=(N-1)*N2-1
      SUXY(M4)=-(UUFEE(N)+X(M3)-SFEE(N2)-UUFEE(M))/(4.*DEL**2)
      M5=N2-1
      DO 6 I=2,M5
    6 SSXY(I)=-(SSFEE(I+1)+X(M4*I-M4)-X(M4*I+M4)
     1     -SSFEE(I-1))/(4.*DEL**2)
      M6=N+1
      N3=2*M4
      CLFEE=BFEE(N)+DEL*(.25*.075493818/.61237244)
     1     *LOGF(1.61237244/.28762756)
      CUFEE=UFEE(N)+BFEE(N)-CLFEE
      SSXY(1)=-(SSFEE(2)+BFEE(M4)-X(N3)-CLFEE)/(4.*DEL**2)
      M7=(N-1)*(N2-1)
      SSXY(N2)=-(CUFEE+X(M7)-UFEE(M4)-SSFEE(M5))/(4.*DEL**2)
      M8=(N-1)*(N2-2)
      N1=(N-1)*N2
      DO33 I=1,M4
      SX(I)=(X(I+M4)-2.*X(I)+BFEE(I))/DEL**2
   33 SX(I+M7)=(X(I+M8)-2.*X(I+M7)+UFEE(I))/DEL**2
      DO 34 I=N,M7
   34 SX(I)=(X(I+M4)-2.*X(I)+X(I-M4))/DEL**2
      DO 35 I=1,M2,M4
      SY(I)=2.*(X(I+1)-X(I))/DEL**2
   35 SXY(I)=0.0
      K=2
      KK=M2+1
    8 DO 36 I=K,KK,M4
   36 SY(I)=(X(I+1)-2.*X(I)+X(I-1))/DEL**2
      IF(K-M)7,9,9
    7 K=K+1
      KK=KK+1
      GO TO 8
```

```
  9 DO 10 I=M4,N1,M4
    J=I/M4
 10 SY(I)=(X(I-1)-2.*X(I)+SFEE(J))/DEL**2
    DO 11 I=2,M
    J=M7+I
    SXY(I)=-(X(I+N)-X(I+M)+BFEE(I-1)-BFEE(I+1))/(4.*DEL**2)
 11 SXY(I+M7)=-(UFEE(I+1)-UFEE(I-1)+X(J-N)-X(J-M))/(4.*DEL**2)
    N3=2*M4-1
    SXY(M4)=-(SFEE(2)+BFEE(M)-X(N3)-BFEE(N))/(4.*DEL**2)
    N4=M7-1
    N5=2*M4
    SXY(N1)=-(-UFEE(M)-SFEE(M5)+X(N4)+UFEE(N))/(4.*DEL**2)
    DO 12 I=N5,M7,M4
    J=I/M4
 12 SXY(I)=-(SFEE(J+1)-SFEE(J-1)+X(I-N)-X(I+M))/(4.*DEL**2)
    K=2+M4
    KK=2+M8
 16 DO 13 I=K,KK,M4
 13 SXY(I)=-(X(I+N)+X(I-N)-X(I+M)-X(I-M))/(4.*DEL**2)
    IF(K-N3)14,15,15
 14 K=K+1
    KK=KK+1
    GO TO 16
 15 PRINT 17
 17 FORMAT(64H    I                   SX                    SY
   1     SXY)
    PRINT 18,(I,(SX(I)),(SY(I)),(SXY(I)),I=1,N1)
 18 FORMAT(I4,3E20.6)
    PRINT 19
 19 FORMAT(42H NUMERICAL BOUNDARY VALUES OF SHEAR STRESS)
    PRINT20,(I,(SBXY(I)),(SUXY(I)),I=1,M4)
 20 FORMAT(I4,2E20.6)
    PRINT21,(I,(SSXY(I)),I=1,N2)
 21 FORMAT(I4,E20.8)
    PRINT 22
 22 FORMAT(39H ACTUAL BOUNDARY VALUES OF SHEAR STRESS)
    PRINT 20,(I,(TBXY(I)),(TUXY(I)),I=1,M4)
    PRINT 21,(I,(TSXY(I)),I=1,N2)
    DO 100 I=1,M4
100 BSX(I)=(X(I)-2.*BFEE(I)+BBFEE(I))/DEL**2
    BSX(N)=(SFEE(1)-2.*BFEE(N)+BBFEE(N))/DEL**2
    DO 200 I=1,N2
    J=M4*I
200 SSY(I)=(X(J)-2.*SFEE(I)+SSFEE(I))/DEL**2
    BSY=(BFEE(M4)-2.*BFEE(N)+SBS)/DEL**2
    USY=(UFEE(M4)-2.*UFEE(N)+SUS)/DEL**2
    PRINT 250
250 FORMAT(25H L. BOUNDARY VALUES OF SX)
    PRINT 255,(I,(BSX(I)),I=1,N)
255 FORMAT(I4,E20.8)
    PRINT 260
260 FORMAT(27H SIDE BOUNDARY VALUES OF SY)
    PRINT 270,BSY
270 FORMAT(7H BSY = E20.8)
```

```
      PRINT 255,(I,(SSY(I)),I=1,N2)
      PRINT 275,USY
  275 FORMAT(7H USY = E20.8)
      END
      SUBROUTINE DISP(DEL,N,N2,X,BFEE,BBFEE,SFEE,SSFEE,
     1   UFEE,UUFEE)
C     SUBROUTINE DISP DETERMINES INTERIOR AND BOUNDARY
C     VALUES OF DISPLACEMENTS
      DIMENSION X(496),BFEE(17),BBFEE(17),SFEE(31),SSFEE(31),
     1   UFEE(17),UUFEE(17),U(496),V(496),VB(17),VS(31),
     2  VU(17),UB(17),US(31),UU(17)
      N1=(N-1)*N2
      M4=N-1
      M6=2*M4
      M=N-2
      DO 100 I=1,N1
      U(I)=0.0
  100 V(I)=0.0
      U(2)= (4./3.)*(X(N)-2.*X(1)+BFEE(1)-X(2)+X(1))/DEL
      DO 105 I=2,M
  105 U(I+1)=((8./3.)*(X(I+M4)-2.*X(I)+BFEE(I))-(4./3.)*
     1    (X(I+1)-2.*X(I)+X(I-1)))/DEL+U(I-1)
      US(1)=((8./3.)*(X(M6)-2.*X(M4)+BFEE(M4))-(4./3.)*
     1(SFEE(1)-2.*X(M4)+X(M)))/DEL+U(M)
      LA=(N-1)*(N2-2)+1
      DO 110 I=N,LA,M4
  110 U(I+1)= (4./3.)*(X(I+M4)-2.*X(I)+X(I-M4)-
     1   X(I+1)+X(I))/DEL
      LB=N+1
      LC=2*M4-1
      LD=LA+1
  119 DO 120 I=LB,LC
  120 U(I+1)=((8./3.)*(X(I+M4)-2.*X(I)+X(I-M4))-(4./3.)*
     1    (X(I+1)-2.*X(I)+X(I-1)))/DEL+U(I-1)
      IF(LB-LD)121,125,125
  121 LB=LB+M4
      LC=LC+M4
      GO TO 119
  125 N3=N2-1
      DO 130 I=2,N3
      J=M4*I
  130 US(I)=((8./3.)*(X(J+M4)-2.*X(J)+X(J-M4))-(4./3.)*
     1    (SFEE(I)-2.*X(J)+X(J-1)))/DEL+U(J-1)
      N4=(N-1)*(N2-1)+1
      N5=N4+1
      N6=N1-1
      U(N5)=(4./3.)*(UFEE(1)-2.*X(N4)+X(LA)-X(N5)+X(N4))/DEL
      N7=(N-1)*(N2-1)
      DO 131 I=N5,N6
  131 U(I+1)=((8./3.)*(UFEE(I-N7)-2.*X(I)+X(I-M4))
     1  -(4./3.)*(X(I+1)-2.*X(I)+X(I-1)))/DEL+U(I-1)
      US(N1)=((8./3.)*(UFEE(M4)-2.*X(N1)+X(N7))
     1  -(4./3.)*(SFEE(N2)-2.*X(N1)+X(N6)))/DEL+U(N6)
      UB(1)=0.0
```

```
      UU(1)=0.0
      UB(2)=(4./3.)*(X(1)-2.*BFEE(1)+BBFEE(1)-BFEE(2)
     1    +BFEE(1))/DEL
      UU(2)=(4./3.)*(UUFEE(1)-2.*UFEE(1)+X(N4)-UFEE(2)
     1    +UFEE(1))/DEL
      DO 135 I=2,M4
      J=I+N7
      UB(I+1)=((8./3.)*(X(I)-2.*BFEE(I)+BBFEE(I))-(4./3.)*
     1    (BFEE(I+1)-2.*BFEE(I)+BFEE(I-1)))/DEL+UB(I-1)
  135 UU(I+1)=((8./3.)*(UUFEE(I)-2.*UFEE(I)+X(J))-(4./3.)*
     1    (UFEE(I+1)-2.*UFEE(I)+UFEE(I-1)))/DEL+UU(I-1)
      V(N)=((8./3.)*2.*(X(2)-X(1))-(4./3.)*(X(N)
     1    -2.*X(1)+BFEE(1)))/DEL
      N8=M6+1
      N9=LA-M4
      DO 140 I=N8,N9,M6
  140 V(I+M4)=((8./3.)*2.*(X(I+1)-X(I))-(4./3.)*(X(I+M4)
     1    -2.*X(I)+X(I-M4)))/DEL+V(I-M4)
      VU(1)=((8./3.)*2.*(X(N5)-X(N4))-(4./3.)*(UFEE(1)
     1    -2.*X(N4)+X(LA)))/DEL+V(LA)
      DO 141 I=1,N
      VB(I)=0.0
  141 VU(I)=0.0
      DO 142 I=1,N2
  142 VS(I)=0.0
      M8=LA+1
      M5=N+1
      M7=M6-2
  149 DO 150 I=M5,M7,2
  150 V(I+1)=-(X(I+N)+X(I-N)-X(I-M)-X(I+M))/DEL
     1    -U(I+M4)+U(I-M4)+V(I-1)
      IF(M5-M8)151,152,152
  151 M5=M5+M6
      M7=M7+M6
      GO TO 149
  152 DO 160 I=2,N3,2
      J=M4*I
  160 VS(I)=-(SFEE(I+1)+X(J-N)-SFEE(I-1)-X(J+M))/DEL
     1   -U(J+M4)+U(J-M4)+V(J-1)
      DO 170 I=3,M,2
      J=N7+I
      VB(I)=((-8./3.)*(X(I+1)-2.*X(I)+X(I-1))+(4./3.)*
     1   (X(I+M4)-2.*X(I)+BFEE(I)))/DEL+V(I+M4)
  170 VU(I)=((8./3.)*(X(J+1)-2.*X(J)+X(J-1))-(4./3.)*
     1    (UFEE(I)-2.*X(J)+X(J-M4)))/DEL+V(J-M4)
      VB(N)=((-8./3.)*(SSFEE(1)-2.*SFEE(1)+X(M4))+(4./3.)*
     1    (SFEE(2)-2.*SFEE(1)+BFEE(N)))/DEL+VS(2)
      L1=N2-1
      VU(N)=((8./3.)*(SSFEE(N2)-2.*SFEE(N2)+X(N1))-(4./3.)*
     1    (UFEE(N)-2.*SFEE(N2)+SFEE(L1)))/DEL+VS(L1)
      PRINT 171
  171 FORMAT(18H INTERIOR U VALUES)
      PRINT 175,(I,(U(I)),I=1,N1)
  175 FORMAT(/4(I6,E15.6))
```

```
      PRINT 180
  180 FORMAT(18H INTERIOR V VALUES)
      PRINT 175,(I,(V(I)),I=1,N1)
      PRINT 185
  185 FORMAT(10H UB VALUES)
      PRINT 190,(I,(UB(I)),I=1,N)
  190 FORMAT(I6,E15.6)
      PRINT 186
  186 FORMAT(10H US VALUES)
      PRINT 190,(I,(US(I)),I=1,N2)
      PRINT 191
  191 FORMAT(10H UU VALUES)
      PRINT 190,(I,(UU(I)),I=1,N2)
      PRINT 195
  195 FORMAT(10H VB VALUES)
      PRINT 190,(I,(VB(I)),I=1,N)
      PRINT 200
  200 FORMAT(10H VS VALUES)
      PRINT 190,(I,(VS(I)),I=1,N2)
      PRINT 205
  205 FORMAT(10H VU VALUES)
      PRINT 190,(I,(VU(I)),I=1,N)
      END
```

APPENDIX IX

GRAPHICAL REPRESENTATION OF THE ANALYTIC AND NUMERICAL CONTINUUM SOLUTIONS

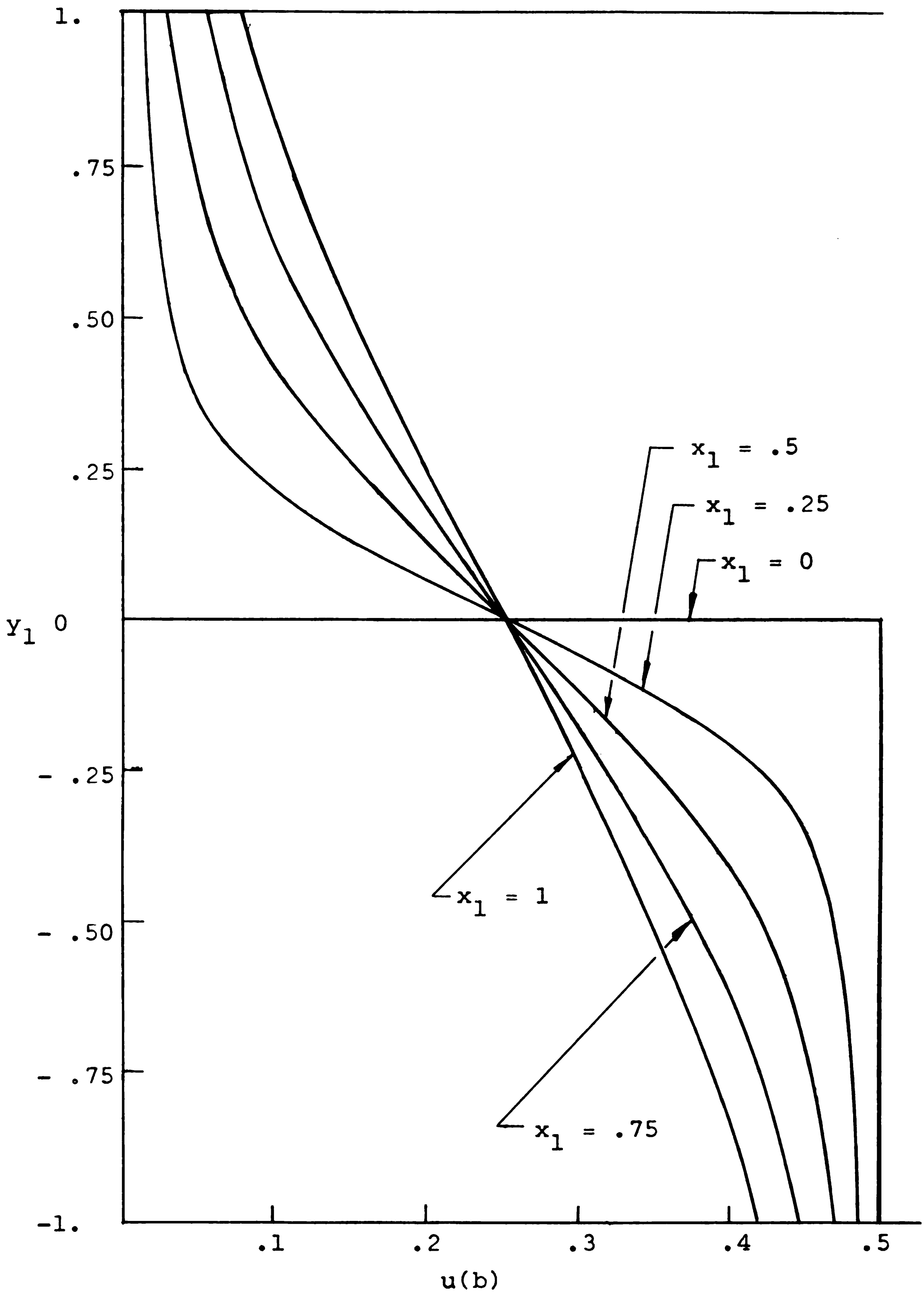

Fig. 34.--u displacement for analytic solution versus y_1

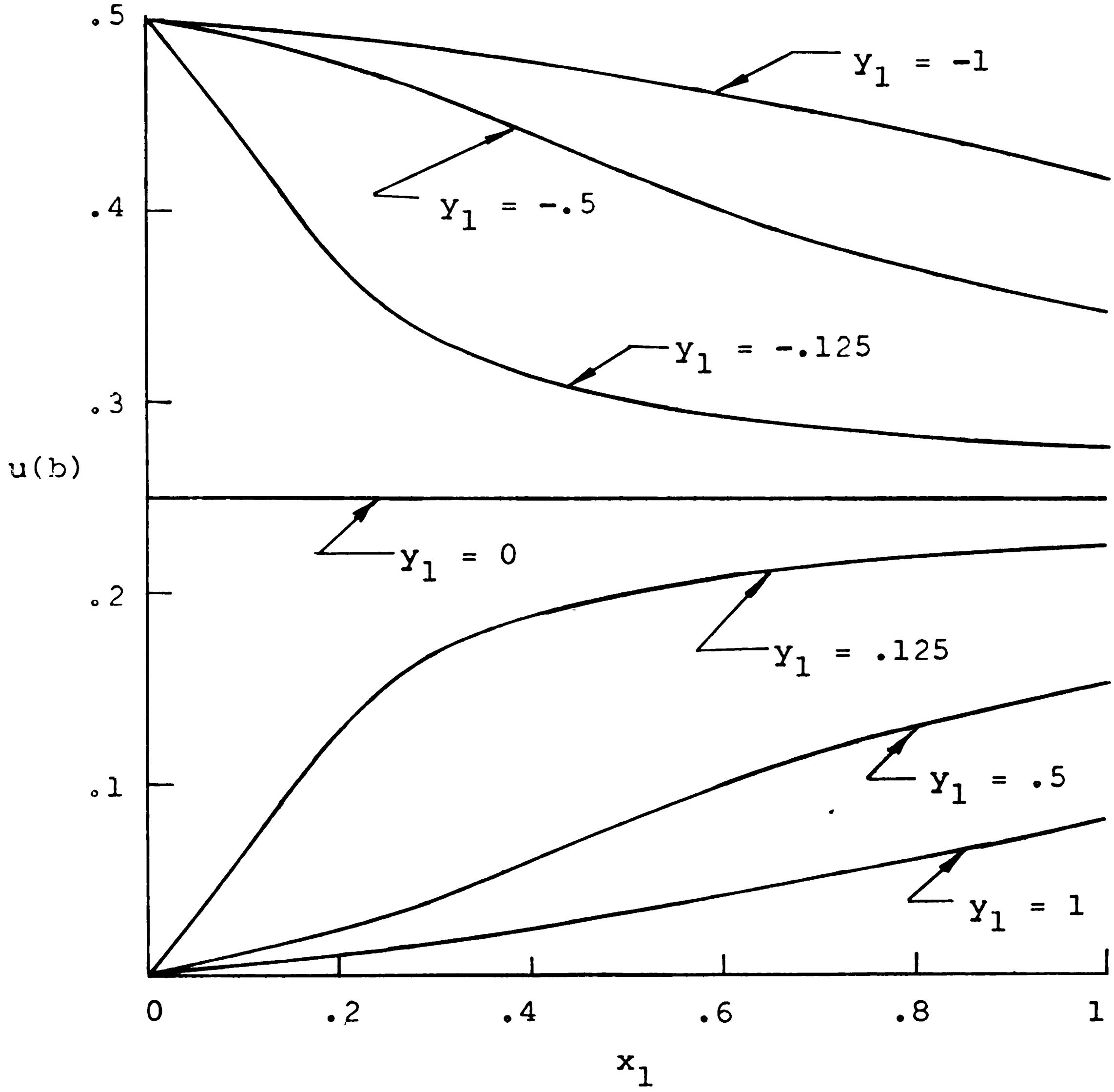

Fig. 35.--u displacement for analytic solution versus x_1

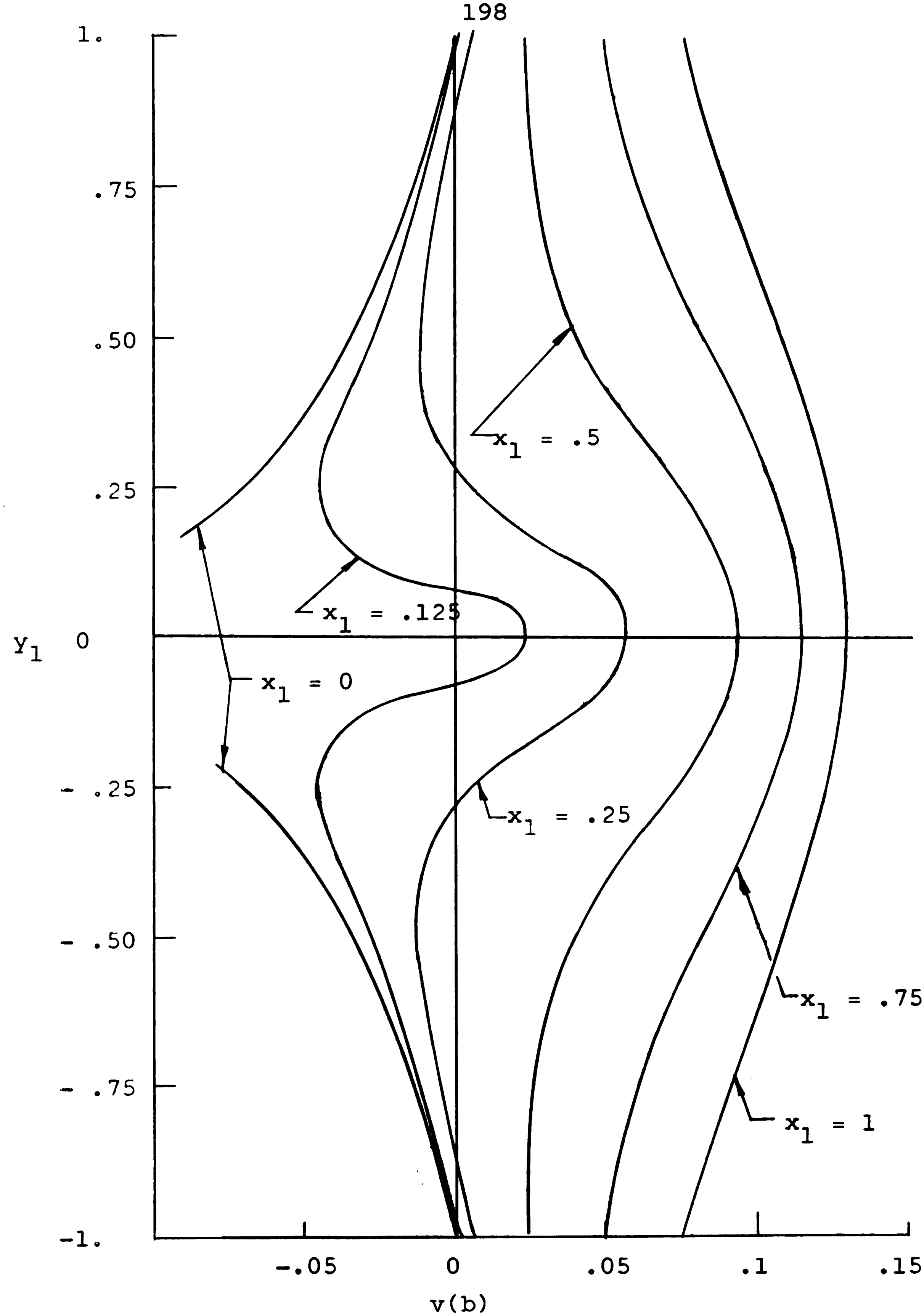

Fig. 36.--v displacement for analytic solution versus y_1

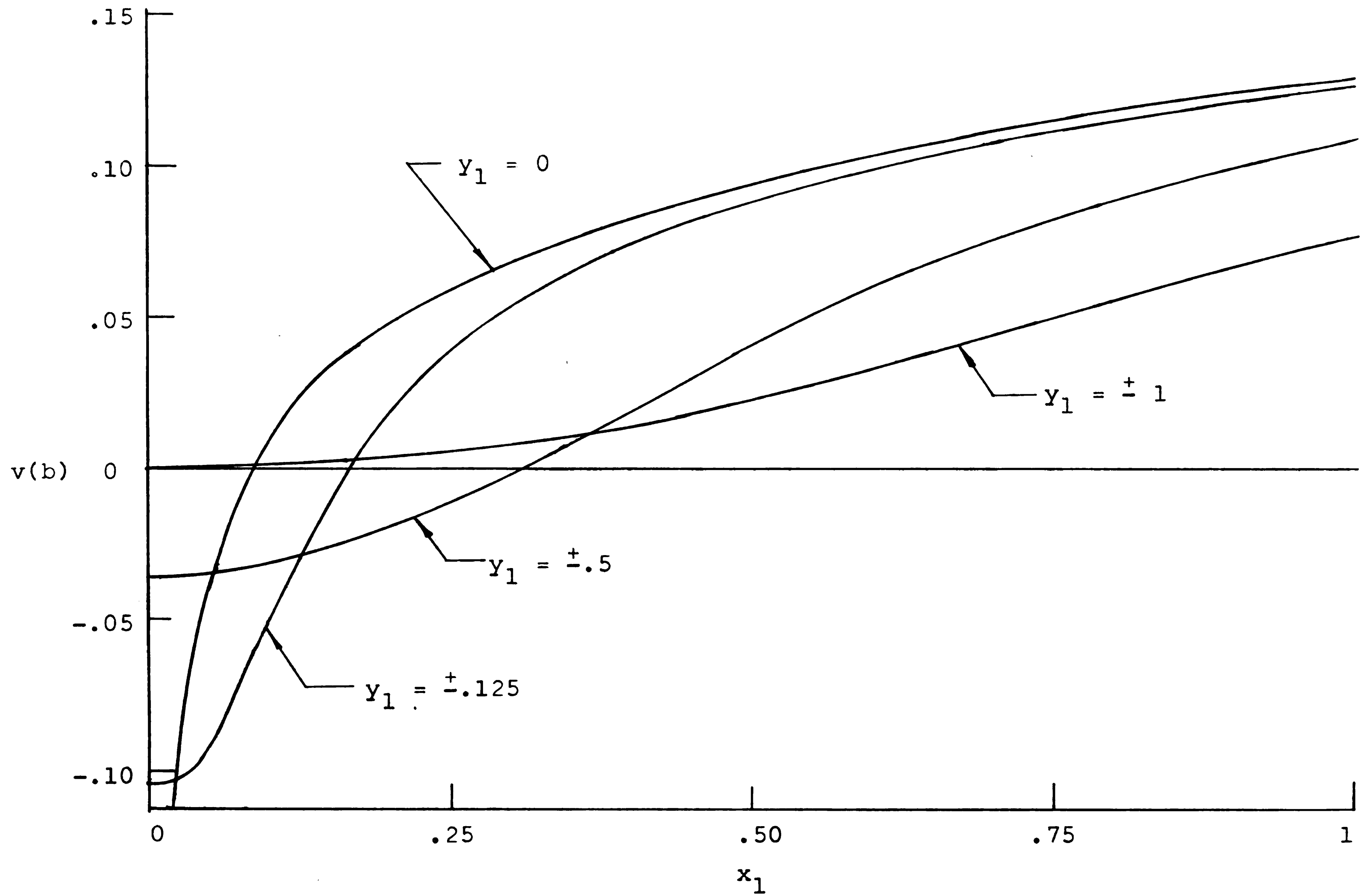

Fig. 37.--v displacement for analytic solution versus x_1

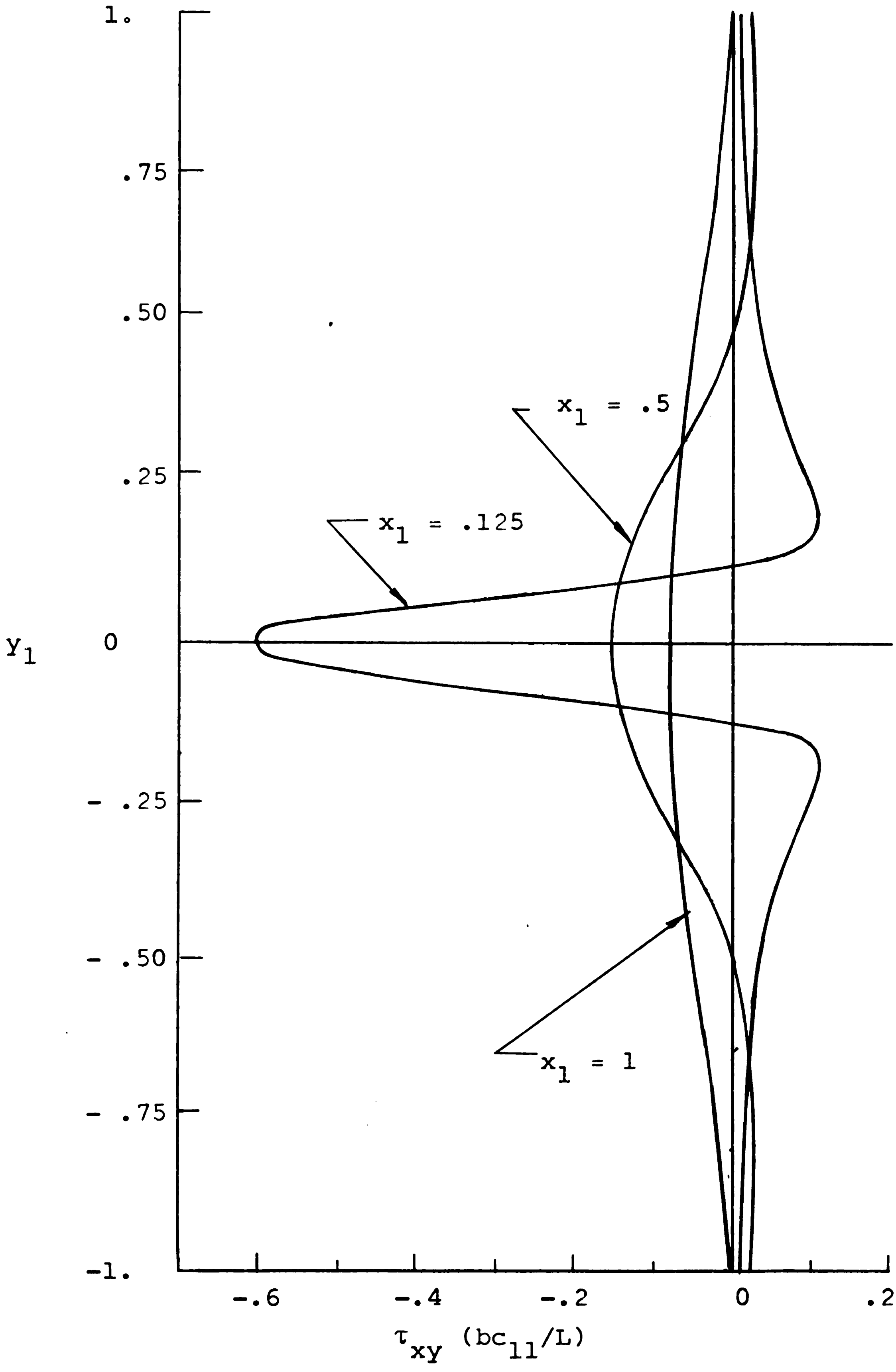

Fig. 38.--τ_{xy} for analytic solution versus y_1

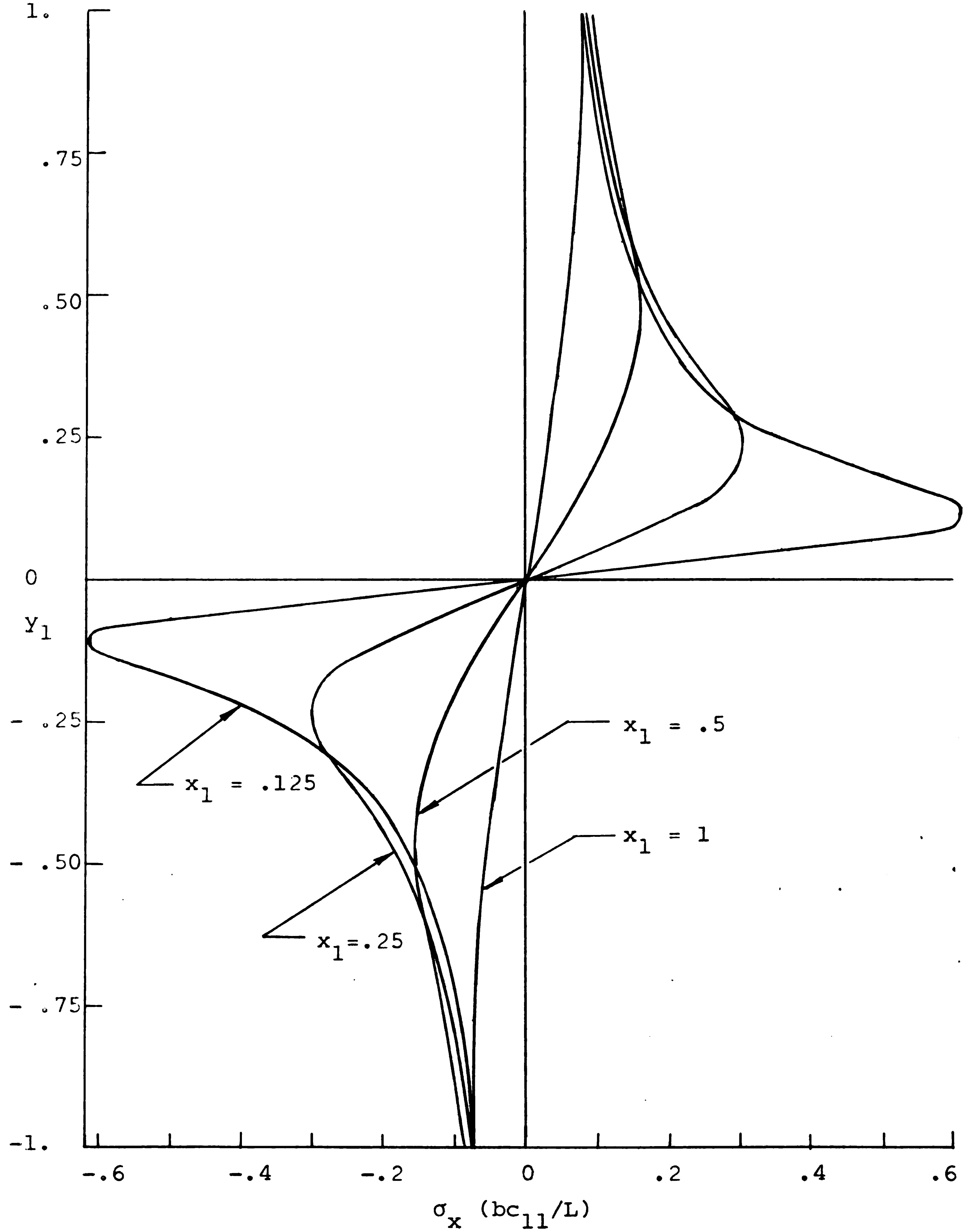

Fig. 39.--σ_x for analytic solution versus y_1

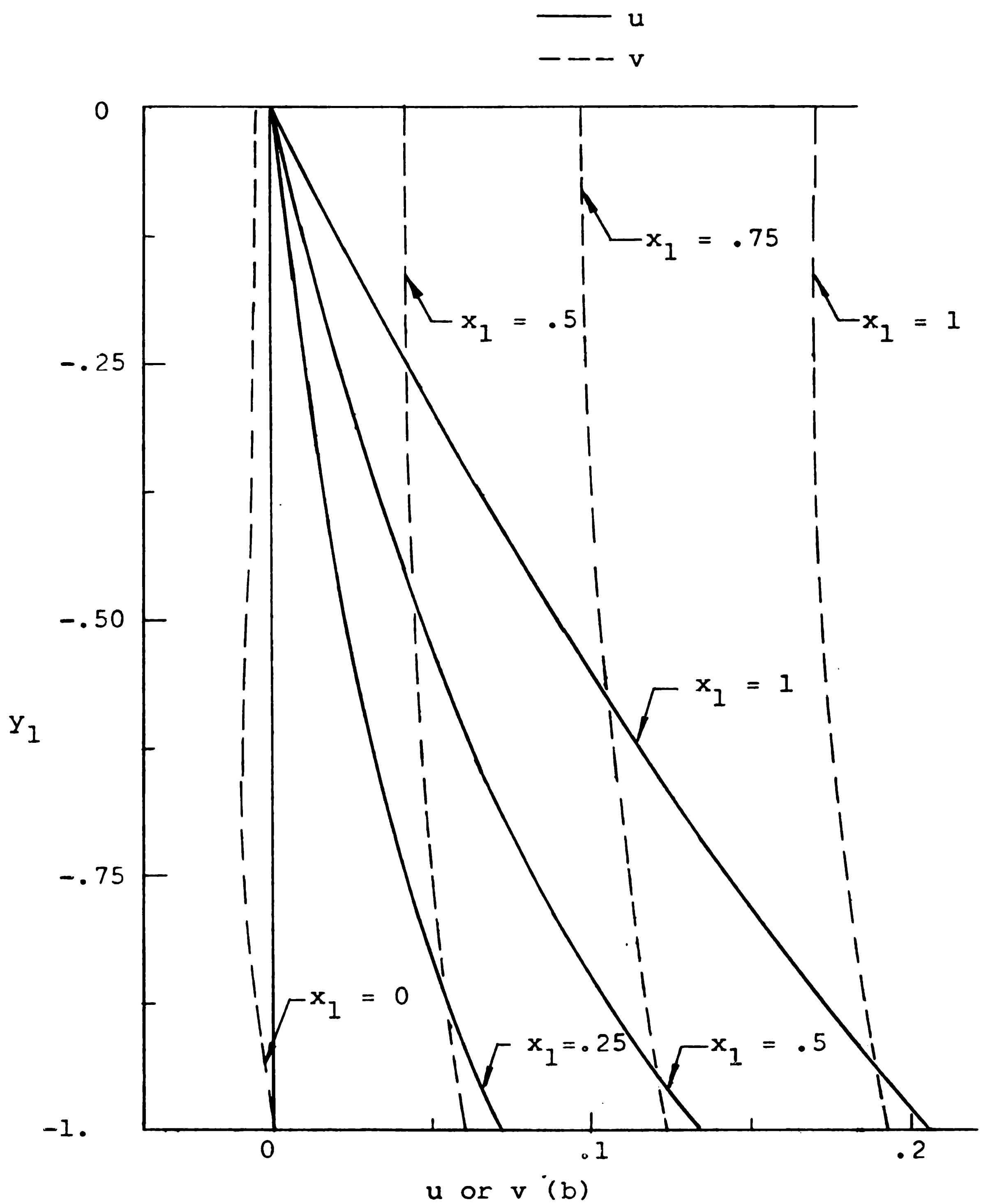

Fig. 40.--u and v displacements for numerical solution versus y_1 (u is antisymmetric and v is symmetric with respect to $y_1 = 0$)

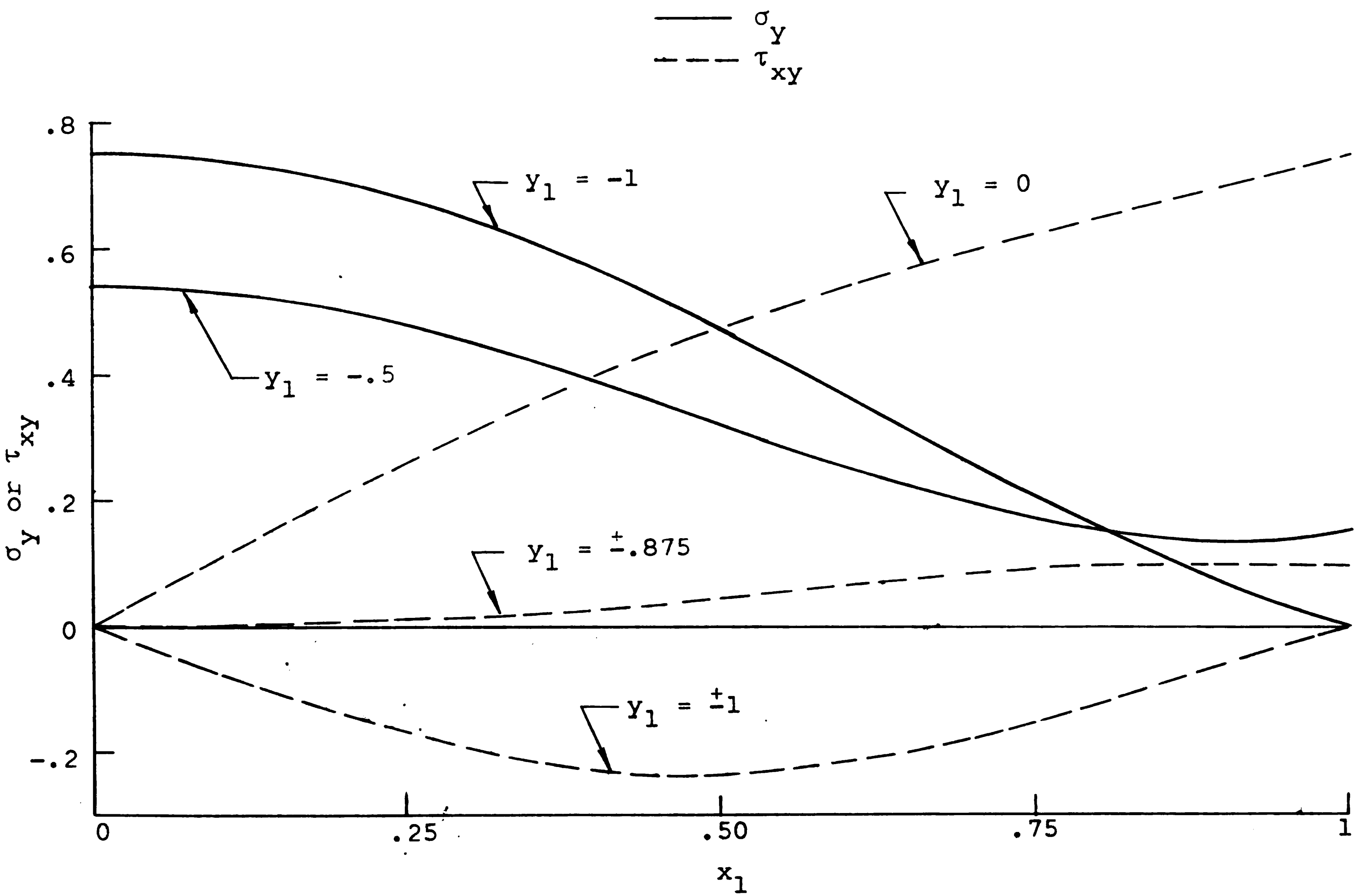

Fig. 41.--σ_y and τ_{xy} for numerical solution versus x_1

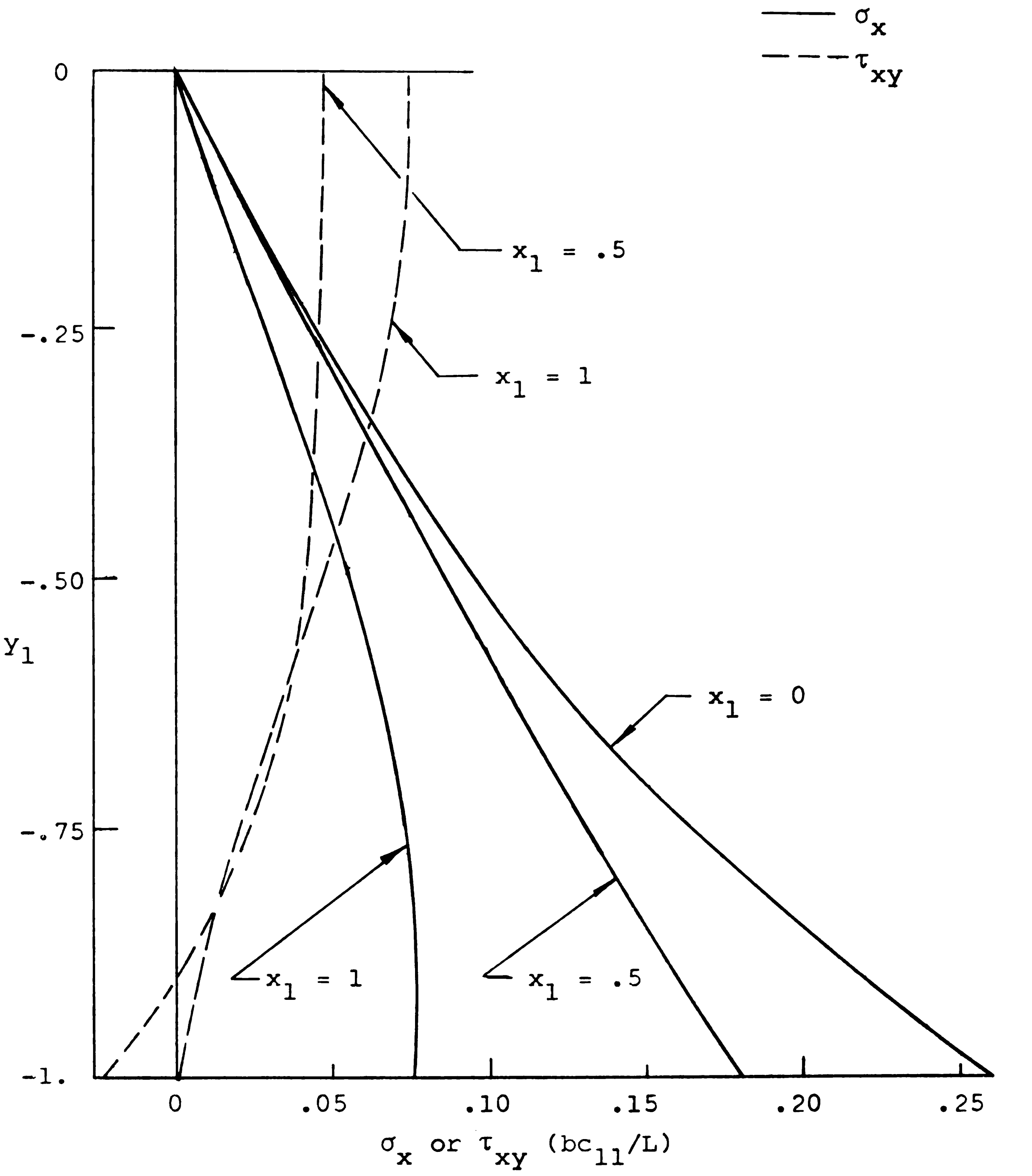

Fig. 42.--σ_x and τ_{xy} for numerical solution versus y_1 (σ_x is antisymmetrical and τ_{xy} is symmetrical with respect to $y_1 = 0$)

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