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SURFACE TOPOGRAPHY OF SINGLE CRYSTALS OF FACE-CENTERED-CUBIC, BODY-CENTERED-CUBIC, SODIUM CHLORIDE, DIAMOND, AND ZINC-BLENDE STRUCTURES

by Robert J. Bacigalupi

Lewis Research Center

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SUMMARY

Atom locations on planes of ideal crystals in face-centered-cubic, body-centered-cubic, sodium chloride, diamond, and zinc-blende structures were obtained on an IBM 7090 computer by quantizing the vector equation of a plane whose orientation is described by the Miller indices. The plotting of solutions results in an orthographic projection of the respective surface plane and several parallel planes immediately adjacent. Surface density, interplanar distance, number of nearest and next nearest neighbors and their locations, nearest surface neighbor distance, and displacement vector are calculated from the atom positions.

INTRODUCTION

Mapping of atom locations on atomically smooth ideal crystal planes is necessary in surface studies, especially for setting up and testing theoretical models of epitaxial growth, and of surface adsorption, desorption, diffusion, and emission. The complexity of geometric mapping methods increases with the plane index in question, and complexity increases the possibility of error. It is this complexity and possibility of error in mapping some cubic crystal planes that prompted the work reported herein. An extension of this program to the calculation of other geometric parameters not mentioned in this report and to other crystal structures (e.g., cesium chloride, calcium fluoride, etc.) is facilitated by the thorough treatment of the fundamental equations.

Plotter programming was done by Grant Carrington through the courtesy of Robert Danek, both of Programming Methods Section, Data Systems Division, Goddard Space Flight Center.

CALCULATION PROCEDURE

A vector equation of a plane is written in terms of the intercepts of that plane with three rectilinear coordinates; the intercepts are reciprocals of the Miller indices

$$\underline{r} = M\underline{u}(1 - s - t) + Ms\underline{v} + Mt\underline{w} \tag{1.3}$$

where $|\underline{u}|$, $|\underline{v}|$, and $|\underline{w}|$ are $1/h$, $1/k$, and $1/l$, respectively, s and t are fractions of the total length of $|\underline{v} - \underline{u}|$ and $|\underline{w} - \underline{u}|$, respectively, and M is a multiplier that expands the area of the plane in question. (A detailed derivation of all equations used in the program appears in appendix A, and the symbols are defined in appendix B.) For zero-index planes

$$\underline{r} = M\underline{u}(1 - s) + Ms\underline{v} + Mt\underline{w}_1 \tag{1.3-0}$$

Four sets of selection rules, one each for face-centered-cubic, body-centered-cubic, diamond, and sodium chloride structures, are written that locate atom sites in the positive octant of the coordinate system.

SELECTION RULES

For face-centered-cubic structures,

$$\underline{r} = \frac{1}{2} n_i \hat{i}_i \qquad \text{where} \quad \sum_i \frac{1}{2} n_i = n_o \tag{2.1}$$

For body-centered-cubic structures,

(A) $$\underline{r} = n_i \hat{i}_i \qquad \text{where} \quad \sum_i n_i = n_o \tag{2.2(A)}$$

(B) $$\underline{r} = \left(\frac{1}{2} + n_i\right)\hat{i}_i \qquad \text{where} \quad \sum_i \left(\frac{1}{2} + n_i\right) = \frac{3}{2} + n_o \tag{2.2(B)}$$

For diamond and zinc-blende structures,

(A) $$\underline{r} = \frac{1}{2} n_i \hat{i}_i \qquad \text{where} \quad \sum_i \frac{1}{2} n_i = n_o \tag{2.3(A)}$$

(B) $$\underline{r} = \left(\frac{1}{4} + \frac{1}{2} n_i\right)\hat{i}_i \qquad \text{where} \quad \sum_i \left(\frac{1}{4} + \frac{1}{2} n_i\right) = \frac{3}{4} + n_o \tag{2.3(B)}$$

Solutions for the zinc-blende structures are identical to solutions for the diamond structures except that, in the zinc-blende structures, the A and B type solutions represent two different elements, whereas in diamond structures they represent the same element.

For sodium chloride structures,

$$\text{(A)} \qquad \underline{r} = \frac{1}{2} n_i \hat{i}_i \qquad \text{where} \quad \sum_i n_i = n_o \qquad (2.4(A))$$

$$\text{(B)} \qquad \underline{r} = \frac{1}{2} n_i \hat{i}_i \qquad \text{where} \quad \sum_i \frac{1}{2} n_i = \frac{1}{2} + n_o \qquad (2.4(B))$$

With the Miller indices as inputs to the first equation, the two equations are solved simultaneously on the IBM 7090 computer by equating parallel components to see where atoms are located on a given plane.

The atom position is read out in terms of s and t, which are transformed into surface coordinates X and Y. From atom positions and the area of the surface plot, the surface density ρ_s is calculated. Of equal interest to the surface physicist are the next few layers of atoms under the surface plane, which (especially in the case of higher index planes) are truly part of the effective surface. Their locations with respect to the surface coordinate system are calculated by adding the appropriate vector $\underline{d}$ perpendicular to the surface and by solving the resulting equations as before.

For face-centered-cubic, body-centered-cubic, and sodium chloride structures, $|d| = \rho_s/\rho_v$. For diamond and zinc-blende structures,

$$|d| = \frac{n_d}{4(h^2 + k^2 + l^2)^{1/2}} \qquad (5d)$$

where $\frac{1}{4(h^2 + k^2 + l^2)^{1/2}}$ is listed in table I as values of $\underline{d}$, and the values for n_d are listed in table VI.

Geometric arrangements of surface atoms and a representative number of underlying planes of atoms are plotted with respect to the surface coordinates, X and Y. Also, surface density ρ_s, interplaner distance $\underline{d}$, number of nearest neighbors CN_1, number of next nearest neighbors CN_2, nearest surface neighbor distance S, and displacement vector $\overline{V}$, are tabulated for planes with Miller indices including all possible combinations of 0, 1, 2, 3, or 4 for the face-centered-cubic, body-centered-cubic, sodium chloride, diamond, and zinc-blende structures. Also, included are selected planes with indices up to 7 in the body-centered-cubic and face-centered-cubic structures. Planes in which the nearest and next nearest neighbors are located are listed in tables II to V. All calculations are performed in terms of the lattice constant a_o so that they may be applied to any crystal in the respective structure.

This mathematically simple method in conjunction with the electronic computer assures accurate results in every case and in an easily usable form. The methods reported herein can be extended to any crystal structure with cubic symmetry (e.g., cesium chloride, calcium fluoride, etc.) by writing the appropriate selection rules.

USE OF TABLES AND PLOTS

The values of S/a and $\overline{V}/a$ are included in table I to allow the reader to extend the plots to any desired area and depth. As mentioned before, the calculations are carried out in units of the lattice constant a_o; therefore, in applying data to a particular crystal, the value of a_o must be inserted appropriately (for surface density divide the value by a_o^2, for all other parameters in table I multiply by a_o). Both coordinates on plots are also in terms of a_o.

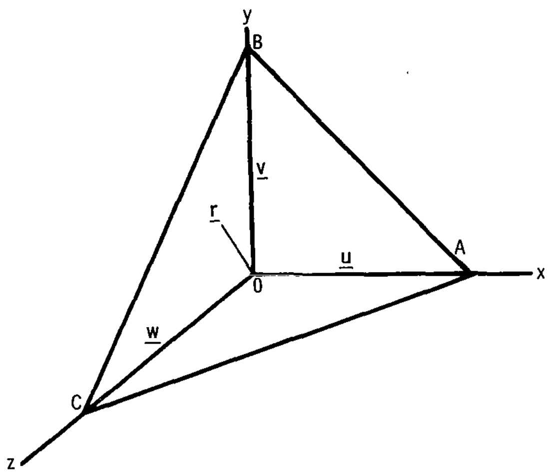
Tables II to V indicate the number of nearest and next nearest neighbors any surface atom has and in which plane (counting from the surface) each one exists. For diamond and zinc-blende structures, the distance between two adjacent planes is not necessarily a constant but is some multiple of d (table I). Table VI indicates the multiples (n_d) of d down from the surface at which planes exist. One must be cautious in interpreting table V for the diamond and zinc-blende structures. The number of the plane in which a neighbor is located, as listed in table V, indicates the number of d's down from the surface and not the number of existent planes down. For example, in the 110 diamond and zinc-blende structures, two nearest neighbors exist in the surface plane and one exists 2d down from the surface; table I shows that 2d down from the surface is the very next plane. In diamond plots, the symbols, of course, refer to the 0^{th}, 1^{st}, 2^{nd}, etc. existent plane from the surface, so it is necessary to use table VI to determine d for each one of the planes.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, January 11, 1964

APPENDIX A

DERIVATION OF EQUATIONS FOR SURFACE ATOM LOCATION

The general equation of a plane is written in terms of the location vector $\underline{r}$ from the origin O in rectilinear coordinates. Sketch (a) shows plane ABC intercepting the x-, y-, and z-axes at A, B, and C, respectively:



(a)

$$AB = |\underline{v} - \underline{u}|$$

$$CB = |\underline{w} - \underline{v}|$$

$$AC = |\underline{w} - \underline{u}|$$

where $\underline{u}$, $\underline{v}$, and $\underline{w}$ represent directed distance along the x-, y-, and z-axes, respectively, to the point of plane-axis interception. Therefore, $|\underline{u}|$, $|\underline{v}|$, and $|\underline{w}|$ also represent the reciprocals of the Miller indices of a crystallographic plane in the cubic system hkl; that is,

$$|\underline{u}| = \frac{1}{h} \qquad |\underline{v}| = \frac{1}{k} \qquad |\underline{w}| = \frac{1}{l}$$

The location vector $\underline{r}$ of any point on plane ABC is given by

$$\underline{r} = \underline{u} + s(\underline{v} - \underline{u}) + t(\underline{w} - \underline{u}) \tag{1.1}$$

where s represents scalar distance along $\underline{v} - \underline{u}$, and t represents scalar distance along $\underline{w} - \underline{u}$. Rearranging equation (1.1) gives

$$\underline{r} = \underline{u}(1 - s - t) + s\underline{v} + t\underline{w} \tag{1.2}$$

For a zero-index plane (e.g., 310), the intercept $\underline{w}$ would be at infinity. This is treated by looking back at the original definition of the vector $|\underline{w} - \underline{u}| \equiv AC$, which in this case is the length of a vector parallel to the z-axis (since $|\underline{w}| = \infty$; $\underline{u}$ is insignificant). In this case, $w \equiv AC$ may be set equal to an arbitrary finite value conveniently large to afford a representative plane.

In order to obtain a usable picture of any given plane, $\underline{u}$, $\underline{v}$, and $\underline{w}$ must be multiplied by a common factor M that merely expands the bounds of the respective plane and thereby includes a larger number of solutions. Because of the varying shapes of the included areas of each plane, M is chosen to suit the respective plane. In the final form equation (1.2) is

$$\underline{r} = M\underline{u}(1 - s - t) + Ms\underline{v} + Mt\underline{w} \tag{1.3}$$

For zero-index planes,

$$\underline{r} = M\underline{u}(1 - s) + Ms\underline{v} + Mt\underline{w}_1 \tag{1.3-0}$$

where $\underline{w}_1$ is a vector whose length is arbitrarily chosen and whose direction is parallel to the axis whose index is zero. The location vector can also be written

$$\underline{r} = \underline{r}_x + \underline{r}_y + \underline{r}_z \tag{2}$$

where $\underline{r}$ locates any atom in the positive octant of a rectilinear coordinate system. But only specific values of $\underline{r}_x$, $\underline{r}_y$, and $\underline{r}_z$ exist for a given crystal structure, and these values are specified by the selection rules given in the following section.

Selection Rules

For face-centered-cubic structures,

$$\left.\begin{aligned} \underline{r}_x &= \frac{1}{2} n_x\hat{i} \\ \underline{r}_y &= \frac{1}{2} n_y\hat{j} \\ \underline{r}_z &= \frac{1}{2} n_z\hat{k} \end{aligned}\right\} \tag{2.1}$$

where

$$\frac{1}{2} n_x + \frac{1}{2} n_y + \frac{1}{2} n_z = n_o$$

where, for all structures, n_i equals any integer from zero the limit of $M|\underline{u}|$, $M|\underline{v}|$, or $M|\underline{w}|$, depending on the respective axis, and n_o equals any integer.

Two selection rules are required for each of the other structures in order to locate all atoms in the lattice. For example, in the body-centered cubic structures, the A selection rule locates unit cell corners, and the B selection rule locates the body-centered-cubic atoms.

For the body-centered-cubic structures,

(A)

$$\left.\begin{aligned} \underline{r}_x &= n_x\hat{i} \\ \underline{r}_y &= n_y\hat{j} \\ \underline{r}_z &= n_z\hat{k} \end{aligned}\right\} \tag{2.2(A)}$$

where

$$n_x + n_y + n_z = n_o$$

(B)

$$\left.\begin{aligned}\underline{r}_x &= \left(\frac{1}{2} + n_x\right)\hat{i}\\ \underline{r}_y &= \left(\frac{1}{2} + n_y\right)\hat{j}\\ \underline{r}_z &= \left(\frac{1}{2} + n_z\right)\hat{k}\end{aligned}\right\} \qquad (2.2(B))$$

where

$$\left(\frac{1}{2} + n_x\right) + \left(\frac{1}{2} + n_y\right) + \left(\frac{1}{2} + n_z\right) = \frac{3}{2} + n_o$$

In the diamond and sodium chloride structures, the A and B type solutions are tagged so that all calculations and plots can be applied to both elemental crystals (e.g., germanium), where A and B types are not distinguishable, and compound crystals (e.g., zinc sulfide), where A and B types represent zinc and sulfur, respectively.

For the diamond and zinc-blende structures,

(A)

$$\left.\begin{aligned}\underline{r}_x &= \frac{1}{2}\, n_x\hat{i}\\ \underline{r}_y &= \frac{1}{2}\, n_y\hat{j}\\ \underline{r}_z &= \frac{1}{2}\, n_z\hat{k}\end{aligned}\right\} \qquad (2.3(A))$$

where

$$\frac{1}{2}\, n_x + \frac{1}{2}\, n_y + \frac{1}{2}\, n_z = n_o$$

(B)

$$\left.\begin{aligned}\underline{r}_x &= \left(\frac{1}{4} + \frac{1}{2}\, n_x\right)\hat{i}\\ \underline{r}_y &= \left(\frac{1}{4} + \frac{1}{2}\, n_y\right)\hat{j}\\ \underline{r}_z &= \left(\frac{1}{4} + \frac{1}{2}\, n_z\right)\hat{k}\end{aligned}\right\} \qquad (2.3(B))$$

where

$$\frac{1}{4} + \frac{1}{2}\, n_x + \frac{1}{4} + \frac{1}{2}\, n_y + \frac{1}{4} + \frac{1}{2}\, n_z = \frac{3}{4} + n_o$$

For the sodium chloride structures,

(A)

$$\left.\begin{aligned} \underline{r}_x &= \frac{1}{2}\, n_x \hat{i} \\ \underline{r}_y &= \frac{1}{2}\, n_y \hat{j} \\ \underline{r}_z &= \frac{1}{2}\, n_z \hat{k} \end{aligned}\right\} \tag{2.4(A)}$$

where

$$\frac{1}{2}\, n_x + \frac{1}{2}\, n_y + \frac{1}{2}\, n_z = n_o$$

(B)

$$\left.\begin{aligned} \underline{r}_x &= \left(\frac{1}{2}\, n_x\right) \hat{i} \\ \underline{r}_y &= \left(\frac{1}{2}\, n_y\right) \hat{j} \\ \underline{r}_z &= \left(\frac{1}{2}\, n_z\right) \hat{k} \end{aligned}\right\} \tag{2.4(B)}$$

where

$$\frac{1}{2}\, n_x + \frac{1}{2}\, n_y + \frac{1}{2}\, n_z = \frac{1}{2} + n_o$$

In order to locate all atoms existing on the plane given by equation (2) within the positive octant specified by the upper limits on n_x, n_y, and n_z, set parallel components of equation (1.3) and (2) equal after the proper selection rule has been inserted into equation (2).

For any given n_o and for any combination of two components (e.g., n_x and n_y) only one value of the third component (n_z) will exist as a solution. This method will work on planes with a zero index only if one of the first two rectilinear components chosen is along the axis that is parallel to the plane.

Since in all cases s and t will appear as fractions of $\overline{AB}$ and $\overline{AC}$, respectively, they must be multiplied by the absolute length of the respective line to be put into terms of the lattice parameter a_o:

$$s' = sM(u^2 + v^2)^{1/2} \tag{3.1}$$

$$t' = tM(u^2 + w^2)^{1/2} \tag{3.2}$$

In the zero-index case,

$$s' = sM(u^2 + v^2)^{1/2} \tag{3.3}$$

$$t' = twM \tag{3.4}$$

where s' and t' are coordinates (not necessarily perpendicular) of the surface plane in units of a_o. Solutions are plotted after transforming from s'- and t'-coordinates into an orthogonal positive X,Y-coordinate system (see figs. 1 to 116):

$$Y = s'(\sin \theta) \tag{3.5}$$

$$X = (u^2 + w^2)^{1/2} - (t' + s' \sin \theta) \tag{3.6}$$

where θ is the angle between s' and t', and

$$\cos \theta = \frac{u^2}{(u^2 + v^2)^{1/2}(u^2 + w^2)^{1/2}} \tag{3.7}$$

SURFACE DENSITY

The surface density is calculated from the locations of the surface solutions (atoms) by counting all solutions (1/2 for the sum of the three triangle vertexes, 1/4 for each rectangle corner, 1/2 for each solution lying on the perimeter of the plot, and 1 for each of the remaining solutions) and dividing by the area of the surface plane:

$$\rho_s = \frac{\text{solutions within plot}}{\text{area of plot in units of } a_o^2} \tag{4a}$$

Since the volume density for face-centered-cubic structures is

$$\rho_v = \frac{4}{a_o^3} \tag{4b}$$

for body-centered-cubic structures is

$$\rho_v = \frac{2}{a_o^3} \tag{4c}$$

and for the sodium chloride structures is

$$\rho_v = \frac{8}{a_o^3} \tag{4d}$$

d can be calculated. For the face-centered-cubic structures,

$$|d| = \frac{\rho_s}{\rho_v} = \frac{\rho_s}{4} \tag{5a}$$

for the body-centered-cubic structures,

$$|d| = \frac{\rho_s}{2} \tag{5b}$$

and for the sodium chloride structures,

$$|d| = \frac{\rho_s}{8} \tag{5c}$$

Since the diamond structure is not fully packed, $d \neq \rho_s/\rho_v$, another method must be used to find d. Assume a simple cubic structure with lattice constant equal to $(1/4)a_o$. This structure will account for all atoms on the diamond structure. Thus, d for the diamond structure must be equal to, or be an integral multiple of, d for the hypothetical simple cubic structure. Therefore,

$$|d| = \frac{n_d}{4(h^2 + k^2 + l^2)^{1/2}} \tag{5d}$$

where n_d may be 1, 2, or 3. Multiples of d are tested in equations (1) and (2) until solutions are found to exist. The n_d necessary to go between the surface and any other plane is recorded in table VI.

Subsequent Planes

The solution for the plane immediately adjacent to the surface may be obtained by adding $\underline{d}$ to equation (1.3). Then, $\underline{d}$ can be factored into x-, y-, and z-components by using the respective direction cosines, or

$$\underline{d} = - \frac{|d|\bar{h}}{(h^2 + k^2 + l^2)^{1/2}} - \frac{|d|\bar{k}}{(h^2 + k^2 + l^2)^{1/2}} - \frac{|d|\bar{l}}{(h^2 + k^2 + l^2)^{1/2}} \tag{6}$$

Parallel components of $\underline{d}$ and equation (1.3) are added, and the resulting equation is solved simultaneously with equation (2), to obtain the location of solutions on the plane immediately beneath the surface in coordinates of the surface. Subsequent planes are obtained by adding $\underline{d}$ again to equation (1.3) for each plane and solving for $\underline{r}$. The location of all atoms in the positive octant is known with respect to the surface plane and its coordinates X and Y.

Surface atom locations and locations of atoms on a few subsequent planes are plotted (after transforming the coordinates from s' and t' to X and and Y) and an orthographic projection of the crystal surface results. Of course, the symmetry of each plane is exactly the same (not necessarily in diamond), but each plane is displaced from the one above it by a displacement vector $\underline{V}$ in the x,y-plane. Only three to five planes need to be plotted to afford a clear representation of the immediate surface vicinity while an infinite number of subsequent planes can be easily extrapolated.

Surface Coordination Numbers

Though only a few planes are plotted, all atom locations down to the $\left[\frac{1}{d}\right]$ plane are retained in the computer memory for further calculations; $\left[\frac{1}{d}\right]$ is the greatest integer function. A typical solution is chosen at or near the centroid of the original surface plot, and the distance R from this typical surface atom to any other atom is known by

$$R = \left[(X_0 - X_i)^2 + (Y_0 - Y_i)^2 + (Id)^2\right]^{1/2} \tag{7}$$

where X_0 and Y_0 are the coordinates of the chosen atom, X and Y of all solutions are in storage, subscript i refers to any given atom, and I indicates the plane in which the i^{th} atom exists (e.g., for surface, I = 0; for plane next to surface, I = 1, etc.).

If R is set equal to the nearest neighbor distance in units of a_o ($1/\sqrt{2}$ for face-centered cubic, $\sqrt{3}/2$ for body-centered cubic, $\sqrt{3}/4$ for diamond, and 1/2 for sodium chloride), the first coordination number CN_1 can be obtained by summing the solutions that satisfy equation (7). Similarly, R is set equal to the next nearest neighbor distance (1 for both face-centered cubic and body-centered cubic, and $\sqrt{2}/2$ for both diamond and sodium chloride) and by summing the number of solutions to equation (7), the second coordination number CN_2 is obtained. For diamond, CN_1 represents the number of remaining tetrahedral bonds. For zinc blende and sodium chloride, where type A and B atoms are distinguishable, CN_1 represents the number of opposite type atoms left touching the chosen surface atom. In the last two cases, CN_2 represents the number of nearest neighbors to a surface atom of the same type. The plane in which each of the neighbors exists is also indicated in tables II to V. The smallest distance between any two atoms of the same type on a given plane is also calculated from equation (7) and is listed in table I as S/a.

The displacement vector $\overline{V}$, which can be drawn from any known atom location to the location of the nearest atom in the very next plane (into the crystal), is calculated by the following equation:

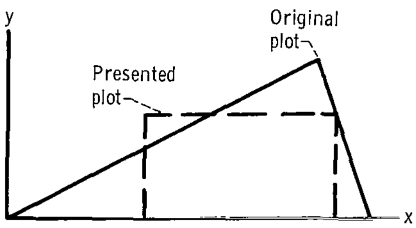
$$\overline{V} = \left[(X_0 - X_1)^2 + (Y_0 - Y_1)^2\right]^{1/2} \tag{8}$$

where X_0 and Y_0 are the coordinates of a chosen atom in the surface plane, and X_1 and Y_1 are the coordinates of the nearest atom in the subsequent plane. The values for X(V), Y(V), and $\overline{V}/a$ are tabulated so that the plot of atom locations may be extrapolated to any extent desired. For diamond and sodium chloride, $\overline{V}/a$ is defined as the vector connecting a surface atom and the closest atom of the same type on the next plane down that contains the chosen type.

Plotting

To ensure accurate computation of coordination numbers and surface densities, the original output plot was allowed to extend to as much as 40 by 30 units. Since all these solutions are not necessary to plot a representative picture of the surface, only representative portions of the original plot are presented, that is, a sufficient number of solution points to show quantitatively how the geometry of each plane is repeated in the plane of the paper and how each plane is displaced by the same vector (not necessarily in diamond) from the plane immediately above it.

It must be remembered that an orthographic view of a slice of the positive octant is plotted, therefore, in all but the zero-index cases the plot of all solutions will be a triangular area, where each successive plane is slightly smaller in area. This means that, at the edges of the triangular plot, some of the solutions on other than the surface plane <u>may</u> be missing; however, more than a sufficient number of solutions appear to indicate clearly what solutions are missing, if any, and their exact position may be determined by extrapolation. When the representative area is plotted, only a portion of the triangle appears in the rectangular plot (sketch (b)), but, as stated before, the empty portion of the plot may easily be filled with the proper solutions by simple extrapolation using $\overline{V}$ and S.



(b)

Every calculation made from the original equations in this program was done on the IBM 7090 computer. The plotting of solutions as they appear was done on a Calcomp digital plotter, which used the output tape from the computer as input and, thereby virtually eliminated the possibility of human error. Note that in the discussion of Selection Rules a special case was made in the program to accommodate planes with indices containing a zero. Further exception would have been necessary for the 100 plane, but for the sake of completeness yet simplicity the plots and calculations for the 100 plane are included but were done manually.

APPENDIX B

SYMBOLS

A,B,C	points of plane-axis interception for x-, y-, and z-axes, respectively
a_o	lattice constant
CN_1	number of nearest neighbors, tables II to V
CN_2	number of next nearest neighbors, tables II to V
d	perpendicular distance between immediately adjacent planes of atoms, table I
h,k,l	Miller indices
$\hat{i},\hat{j},\hat{k}$	unit vectors in x-, y-, and z-directions
M	factor for expanding plane areas
n_d	for diamond and zinc blende only, multiple of d (table I) giving true distance between surface and existing planes, table VI
n_o	integral values of sum of n_x, n_y, and n_z that follow selection rule for respective structure
n_x,n_y,n_z	integral values of a_o in x-, y-, and z-directions, respectively
R	distance from surface atom to any other atom in crystal
$\underline{r}$	location vector of plane
S	vector locating nearest atom to any atom of same type on same plane, table I
s,t	fractional length of $\overline{AB}$ and $\overline{AC}$, respectively
s',t'	length of s and t in terms of a_o
$\underline{u},\underline{v},\underline{w}$	location vectors of x-, y-, and z-intercepts, respectively, of given plane
$\overline{V}$	vector which if drawn from any known atom location will locate (in x,y-plane) an atom of same type on plane immediately below it, table I
X,Y	coordinates of surface plane, figs. 1 to 116
x,y,z	coordinates in sketch (a)

$X(V)$	X-component of $\overline{V}$, table I
$Y(V)$	Y-component of $\overline{V}$, table I
θ	angle between s' and t'
ρ_s	surface density, table I
ρ_v	volume density

TABLE I. - SURFACE PARAMETERS

Structure	Plane, hkl	Surface density $\times a_o^2$	d/a_o	Coordination number (1)	Coordination number (2)	$X(V)/a_o$	$Y(V)/a_o$	$\overline{V}/a_o$	S/a_o
FCC	100	2.00000	0.50000	8	5	0.	0.50000	0.50000	0.70711
FCC	110	1.41421	0.35355	7	4	0.50000	0.35355	0.61237	0.70711
FCC	111	2.30940	0.57735	9	3	0.	0.40825	0.40825	0.70711
FCC	210	0.89443	0.22361	6	4	0.	0.67082	0.67082	1.00000
FCC	211	0.81650	0.20412	7	3	0.22361	0.63901	0.67700	0.70711
FCC	221	0.66667	0.16667	7	3	0.44721	0.52175	0.68718	0.70711
FCC	310	0.63246	0.15811	6	4	0.50000	0.47434	0.68920	1.00000
FCC	320	0.55470	0.13868	6	4	0.	0.69338	0.69338	1.00000
FCC	311	1.20605	0.30151	7	3	0.63246	0.09535	0.63960	0.70711
FCC	321	0.53452	0.13363	6	3	0.15811	0.67612	0.69437	1.22474
FCC	322	0.48507	0.12127	7	3	0.69338	0.06727	0.69663	0.70711
FCC	331	0.91766	0.22942	7	3	0.47434	0.47156	0.66886	0.70711
FCC	332	0.42640	0.10660	7	3	0.69338	0.08870	0.69903	0.70711
FCC	410	0.48507	0.12127	6	4	0.50000	0.48507	0.69663	1.00000
FCC	430	0.40000	0.10000	6	4	0.	0.70000	0.70000	1.00000
FCC	411	0.47140	0.11785	7	3	1.09141	0.54308	1.21906	0.70711
FCC	421	0.43644	0.10911	6	3	0.48507	0.50279	0.69864	1.22474
FCC	431	0.39223	0.09806	6	3	0.12127	0.68969	0.70027	1.58114
FCC	432	0.37139	0.09285	6	3	0.44721	0.53980	0.70098	1.22474
FCC	433	0.34300	0.08575	7	3	0.70000	0.05145	0.70189	0.70711
FCC	443	0.31235	0.07809	7	3	0.70000	0.06247	0.70278	0.70711
FCC	441	0.34816	0.08704	7	3	1.45521	0.61219	1.57874	0.70711
FCC	510	0.39223	0.09806	6	4	0.50000	0.49029	0.70027	1.00000
FCC	511	0.76980	0.19245	7	3	0.49029	0.47178	0.68041	0.70711
FCC	540	0.31235	0.07809	6	4	0.	0.70278	0.70278	1.00000
FCC	554	0.24618	0.06155	7	3	0.70278	0.04806	0.70442	0.70711
FCC	551	0.56011	0.14003	7	3	0.98058	0.13731	0.99015	0.70711
FCC	543	0.28284	0.07071	6	3	0.25725	0.65485	0.70356	1.22474
FCC	610	0.32880	0.08220	6	4	0.50000	0.49320	0.70231	1.00000
FCC	611	0.32444	0.08111	7	3	1.56179	1.02676	1.86907	0.70711
FCC	650	0.25607	0.06402	6	4	0.	0.70420	0.70420	1.00000
FCC	665	0.20307	0.05077	7	3	0.70420	0.03900	0.70528	0.70711
FCC	661	0.23408	0.05852	7	3	2.54818	0.05772	2.54884	0.70711
FCC	654	0.22792	0.05698	6	3	0.27735	0.64794	0.70481	1.22474
FCC	711	0.56011	0.14003	7	3	0.49497	0.48517	0.69310	0.70711
FCC	771	0.40202	0.10050	7	3	0.98995	0.09949	0.99494	0.70711
BCC	100	1.00000	0.50000	4	5	0.50000	0.50000	0.70711	1.00000
BCC	110	1.41421	0.70711	6	4	0.50000	0.	0.50000	0.86603
BCC	111	0.57735	0.28868	4	3	0.70711	0.40825	0.81650	1.41421
BCC	210	0.44721	0.22361	4	4	0.50000	0.67082	0.83666	1.00000
BCC	211	0.81650	0.40825	5	3	0.67082	0.36515	0.76376	0.86603
BCC	221	0.33333	0.16667	4	3	0.22361	0.81989	0.84984	1.41421
BCC	310	0.63246	0.31623	4	4	0.50000	0.63246	0.80623	1.00000
BCC	320	0.27735	0.13868	4	4	0.50000	0.69338	0.85485	1.00000
BCC	311	0.30151	0.15076	4	3	0.63246	0.57208	0.85280	1.41421
BCC	321	0.53452	0.26726	5	3	0.31623	0.76064	0.82375	0.86603
BCC	322	0.24254	0.12127	4	3	0.69338	0.50450	0.85749	1.41421
BCC	331	0.22942	0.11471	4	3	0.31623	0.79802	0.85840	1.41421
BCC	332	0.42640	0.21320	4	3	0.13868	0.82784	0.83937	1.41421
BCC	410	0.24254	0.12127	4	4	0.50000	1.57648	1.65387	1.00000
BCC	430	0.20000	0.10000	4	4	0.50000	0.70000	0.86023	1.00000
BCC	411	0.47140	0.23570	4	3	0.60634	0.57166	0.83333	1.41421
BCC	421	0.21822	0.10911	4	3	0.60634	0.60864	0.85912	2.23607
BCC	431	0.39223	0.19612	5	3	0.36380	0.76104	0.84353	0.86603
BCC	432	0.18570	0.09285	4	3	0.67082	0.53980	0.86103	2.23607
BCC	433	0.34300	0.17150	4	3	0.70000	0.48020	0.84887	1.41421
BCC	443	0.15617	0.07809	4	3	1.50000	0.70278	1.65647	1.41421
BCC	441	0.17408	0.08704	4	3	0.36380	0.78107	0.86164	1.41421
BCC	510	0.39223	0.19612	4	4	0.	0.98058	0.98058	1.00000
BCC	511	0.19245	0.09623	4	3	1.56893	0.52840	1.65552	1.41421
BCC	540	0.15617	0.07809	4	4	0.50000	0.70278	0.86250	1.00000
BCC	554	0.24618	0.12309	4	3	1.40556	0.09612	1.40885	1.41421
BCC	551	0.14003	0.07001	4	3	0.39223	0.76893	0.86319	1.41421
BCC	543	0.28284	0.14142	4	3	0.68599	0.50932	0.85440	1.65831
BCC	610	0.16440	0.08220	4	4	0.50000	2.54818	2.59678	1.00000
BCC	611	0.32444	0.16222	4	3	0.	0.98675	0.98675	1.41421
BCC	650	0.12804	0.06402	4	4	0.50000	0.70420	0.86366	1.00000
BCC	665	0.10153	0.05077	4	3	2.24065	1.93053	2.95760	1.41421
BCC	661	0.11704	0.05852	4	3	0.41100	0.76004	0.86405	1.41421
BCC	654	0.11396	0.05698	4	3	1.52543	0.64794	1.65733	2.44949
BCC	711	0.14003	0.07001	4	3	1.55563	1.52483	2.17832	1.41421
BCC	771	0.10050	0.05025	4	3	0.42426	0.75331	0.86457	1.41421

TABLE I. - Concluded. - SURFACE PARAMETERS

Structure	Plane, hkl	Surface density $\times a_o^2$	d/a_o	Coordination number		$X(V)/a_o$	$Y(V)/a_o$	$\overline{V}/a_o$	S/a_o
				(1)	(2)				
NA CL	100	4.00000	0.50000	5	8	0.50000	0.	0.50000	0.70711
NA CL	110	2.82843	0.35355	4	7	0.50000	0.35355	0.61237	0.70711
NA CL	111	2.3094C	0.28868	3	9	0.	C.40825	0.40825	0.70711
NA CL	210	1.78885	0.22361	4	6	0.	0.67082	0.67082	1.00000
NA CL	211	1.63299	0.20412	3	7	0.22361	0.63901	0.67700	0.70711
NA CL	221	1.33333	0.16667	3	7	0.44721	0.52175	0.68718	0.70711
NA CL	310	1.26491	0.15811	4	6	0.50000	C.47434	0.68920	1.000CC
NA CL	320	1.10940	0.13868	4	6	0.	0.69338	0.69338	1.00000
NA CL	311	1.20605	0.15076	3	7	0.63246	0.09535	0.63960	0.70711
NA CL	321	1.06904	0.13363	3	6	0.15811	0.67612	0.69437	1.22474
NA CL	322	C.97C14	0.12127	3	7	0.69338	0.06727	C.69663	C.70711
NA CL	332	0.85280	0.10660	3	7	0.69338	0.08870	0.69903	0.70711
NA CL	331	0.91766	0.11471	3	7	0.47434	0.47156	0.66886	0.70711
NA CL	410	0.97014	0.12127	4	6	0.50000	0.48507	0.69663	1.00000
NA CL	430	C.80CCC	0.10000	4	6	0.	0.70000	0.70000	1.00000
NA CL	411	0.94281	0.11785	3	7	1.09141	0.54308	1.21906	0.70711
NA CL	421	0.87287	0.10911	3	6	0.48507	0.50279	0.69864	1.22474
NA CL	431	C.78446	0.09806	3	6	C.12127	0.68969	C.70027	1.58114
NA CL	432	C.74278	0.09285	3	6	0.44721	0.53980	0.70098	1.22474
NA CL	433	0.68599	0.08575	3	7	0.70000	0.05145	0.70189	0.70711
NA CL	443	0.62470	0.07809	3	7	0.70000	0.06247	0.70278	0.70711
NA CL	441	C.69631	0.C8704	3	7	1.57648	0.08444	1.57874	0.70711
DIA.	100	2.00000	0.25000	2	8	0.	0.50000	0.50000	0.70711
DIA.	110	2.82843	0.17678	3	7	0.50000	0.35355	0.61237	0.70711
DIA.	111	2.30940	0.14434	3	9	0.00000	0.40825	0.40825	0.70711
DIA.	210	.89443	0.1118C	2	6	0.	0.67082	0.67082	1.00000
DIA.	211	1.76908	0.10206	3	7	0.22361	0.63901	0.67700	0.70711
DIA.	221	.66667	0.08333	3	7	0.44721	0.52175	0.68718	0.70711
DIA.	310	1.26491	0.07906	2	6	0.50000	0.47434	0.68920	1.00000
DIA.	320	.55470	0.C6934	2	6	0.	0.69338	0.69338	1.00000
DIA.	311	1.20604	0.07538	2	7	0.63246	0.09535	0.63960	0.70711
DIA.	321	1.03935	0.06682	3	6	0.15811	0.67612	0.69437	1.22474
DIA.	322	.48507	0.06063	3	7	0.69338	0.06727	0.69663	0.70711
DIA.	332	.78174	0.C5330	3	7	0.69338	0.08870	0.69903	0.70711
DIA.	331	.91766	0.05735	3	7	0.47434	0.47156	0.66886	0.70711
DIA.	410	.48507	0.06063	2	6	0.50000	0.48507	0.69663	1.00000
DIA.	430	.40000	0.05000	2	6	0.	0.70000	0.70000	1.00000
DIA.	411	.86424	0.05893	2	7	1.09141	0.54308	1.21906	0.70711
DIA.	421	.43644	0.05455	2	6	0.48507	0.50279	0.69864	1.22474
DIA.	431	.84984	0.04903	3	6	0.12127	0.68969	0.70027	1.58114
DIA.	432	.37139	0.04642	3	6	0.44721	0.53980	0.70098	1.22474
DIA.	433	.74316	0.04287	3	7	0.70000	0.05145	0.70189	0.70711
DIA.	443	.31235	0.03904	3	7	0.70000	0.06247	0.70278	0.70711
DIA.	441	.34815	0.04352	3	7	1.45521	0.61219	1.57874	0.70711

TABLE II. - LOCATION OF NEAREST NEIGHBOR

FOR FACE-CENTERED-CUBIC STRUCTURE

(a) Nearest neighbor distance, 0.707107

Plane, hkl	Plane in which neighbors exist, counting from surface plane																		Total
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
100	4	4																	8
110	2	4	1																7
111	6	3																	9
210		3	2	1															6
211	2	2	1	2															7
221	2	2		2	1														7
310		2	1	2	1														6
320		1	2	2		1													6
311	2	3	2																7
321		2	1	1	1	1													6
322	2	2			1	2													7
331	2	2	2	1															7
332	2	2				2	1												7
410		2		1	2	1													6
430		1		2	2			1											6
411	2		1	2		2													7
421		1	1	2		1	1												6
431		1	1	1	1	1		1											6
432		2	1			1	1	1											6
433	2	2					1	2											7
443	2	2						2	1										7
441	2			2		2			1										7
510		2			1	2	1												6
511	2	1	2	2															7
540		1			2	2				1									6
554	2	2								2	1								7
551	2		2	2		1													7
543		2	1					1	1	1									6
610		2				1	2	1											6
611	2		1			2		2											7
650		1				2	2					1							6
665	2	2										2	1						7
661	2					2		2					1						7
654		2	1							1	1	1							6
711	2	1		2	2														7
771	2			2	2			1											7

TABLE II. - Concluded. LOCATION OF NEXT NEAREST NEIGHBOR

FOR FACE-CENTERED-CUBIC STRUCTURE

(b) Next nearest neighbor distance, 1.00000

Plane, hkl	Plane in which neighbors exist, counting from surface plane																		Total
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
100	4		1																5
110	2		2																4
111		3																	3
210	2		1		1														4
211			2		1														3
221			1		2														3
310	2		1				1												4
320	2				1		1												4
311		2		1															3
321			1		1		1												3
322					2		1												3
331		1		2															3
332					1		2												3
410	2		1						1										4
430	2						1		1										4
411			2						1										3
421			1		1				1										3
431			1				1		1										3
432					1		1		1										3
433							2		1										3
443							1		2										3
441			1						2										3
510	2		1								1								4
511		2				1													3
540	2								1		1								4
554									1		2								3
551		1				2													3
543							1		1		1								3
610	2		1										1						4
611			2										1						3
650	2										1		1						4
665											1		2						3
661			1										2						3
654									1		1		1						3
711		2						1											3
771		1						2											3

TABLE III. - LOCATION OF NEAREST NEIGHBOR FOR BODY-CENTERED-CUBIC STRUCTURE

(a) Nearest neighbor distance, 0.866025

Plane, hkl	Plane in which neighbors exist, counting from surface plane																		Total
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
100	0	4																	4
110	4	2																	6
111		3		1															4
210		2		2															4
211	2	2	1																5
221		2		1		1													4
310		2	2																4
320		2				2													4
311		1		2		1													4
321	2	1	1	1															5
322		1		2				1											4
331		2				1		1											4
332		2	1		1														4
410				2		2													4
430		2						2											4
411		1	2	1															4
421		1		1		1		1											4
431	2	1		1	1														5
432		1		1		1				1									4
433		1	2			1													4
443				2		1						1							4
441		2						1		1									4
510			2	2															4
511				1		2		1											4
540		2								2									4
554			2	1				1											4
551		2								1		1							4
543		1	1	1			1												4
610						2		2											4
611			1	2	1														4
650		2										2							4
665						2		1										1	4
661		2										1		1					4
654				1		1		1								1			4
711						1		2		1									4
771		2												1		1			4

TABLE III. - Concluded. LOCATION OF NEXT NEAREST NEIGHBOR FOR BODY-CENTERED-CUBIC STRUCTURE

(b) Next nearest neighbor distance, 1.00000

Plane, hkl	Plane in which neighbors exist, counting from surface plane																		Total
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
100	4		1																5
110	2	2																	4
111			3																3
210	2		1		1														4
211		2	1																3
221			1		2														3
310	2	1		1															4
320	2				1		1												4
311			2				1												3
321		1	1	1															3
322					2		1												3
331			1				2												3
332			1	2															3
410	2		1						1										4
430	2						1		1										4
411		2			1														3
421			1		1				1										3
431		1		1	1														3
432					1		1		1										3
433				2	1														3
443							1		2										3
441			1						2										3
510	2	1				1													4
511			2								1								3
540	2								1		1								4
554					1	2													3
551			1								2								3
543				1	1	1													3
610	2		1										1						4
611		2					1												3
650	2										1		1						4
665											1		2						3
661			1										2						3
654									1		1		1						3
711			2												1				3
771			1												2				3

TABLE IV. - LOCATION OF NEAREST AND NEXT NEAREST NEIGHBORS

FOR SODIUM CHLORIDE STRUCTURE

(a) Nearest neighbor distance, 0.500000

Plane, hkl	Plane in which neighbors exist, counting from surface plane																		Total
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
100	4	1																	5
110	2	2																	4
111		3																	3
210	2	1	1																4
211		2	1																3
221		1	2																3
310	2	1		1															4
320	2		1	1															4
311		2		1															3
321		1	1	1															3
322			2	1															3
331		1		2															3
332			1	2															3
410	2	1			1														4
430	2			1	1														4
411		2			1														3
421		1	1		1														3
431		1		1	1														3
432			1	1	1														3
433				2	1														3
443				1	2														3
441		1			2														3
(b) Next nearest neighbor distance, 0.707107																			
100	4	4																	8
110	2	4	1																7
111	6		3																9
210		3	2	1															6
211	2	2	1	2															7
221	2	2		2	1														7
310		2	1	2	1														6
320		1	2	2		1													6
311	2		3		2														7
321		2	1	1	1	1													6
322	2	2			1	2													7
331	2		2		2		1												7
332	2	2				2	1												7
410		2		1	2	1													6
430		1		2	2			1											6
411	2		1	2		2													7
421		1	1	2		1	1												6
431		1	1	1	1	1		1											6
432		2	1			1	1	1											6
433	2	2					1	2											7
443	2	2						2	1										7
441	2			2		2			1										7

TABLE V. - LOCATION OF NEAREST AND NEXT NEAREST NEIGHBORS

FOR DIAMOND STRUCTURE

(a) Nearest neighbor distance, 0.433013

Plane, hkl	Plane in which neighbors exist, counting from surface plane																		Total
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	
100	0	2																	2
110	2		1																3
111		3																	3
210		1		1															2
211	1		2																3
221		2		1															3
310			1		1														2
320		1				1													2
311				2															2
321	1		1		1														3
322		1		2															3
331		2				1													3
332			2		1														3
410				1		1													2
430		1						1											2
411					2														2
421				1		1													2
431	1		1				1												3
432		1		1		1													3
433			1		2														3
443				2		1													3
441		2						1											3

(b) Next nearest neighbor distance, 0.707107

Plane, hkl	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	Total
100	4	4																	8
110	2		4		1														7
111	6				3														9
210			3		2		1												6
211	2		2		1		2												7
221	2		2				2		1										7
310			2		1		2		1										6
320			1		2		2				1								6
311	2				3				2										7
321			2		1		1		1		1								6
322	2		2						1		2								7
331	2				2				2				1						7
332	2		2								2		1						7
410			2				1		2		1								6
430			1				2		2						1				6
411	2				1		2				2								7
421			1		1		2				1		1						6
431			1		1		1		1		1				1				6
432			2		1						1		1		1				6
433	2		2										1		2				7
443	2		2												2		1		7
441	2						2				2						1		7

TABLE VI. - LOCATION OF POPULATED PLANES IN THE DIAMOND STRUCTURE

Plane, hkl	Multiples of d necessary to locate plane												
	0	1	2	3	4	5	6	7	8	9	10	11	12
100	*	*	*	*	*	*	*	*	*	*	*	*	*
110	*		*		*		*		*		*		*
111	*	*			*	*			*	*			*
210	*	*	*	*	*	*	*	*	*	*	*	*	*
211	*		*		*		*		*		*		*
221	*	*	*	*	*	*	*	*	*	*	*	*	*
310	*		*		*		*		*		*		*
320	*	*	*	*	*	*	*	*	*	*	*	*	*
311	*			*	*			*	*			*	*
321	*		*		*		*		*		*		*
322	*	*	*	*	*	*	*	*	*	*	*	*	*
332	*		*		*		*		*		*		*
331	*	*			*	*			*	*			*
410	*	*	*	*	*	*	*	*	*	*	*	*	*
430	*	*	*	*	*	*	*	*	*	*	*	*	*
411	*		*		*		*		*		*		*
421	*	*	*	*	*	*	*	*	*	*	*	*	*
431	*		*		*		*		*		*		*
432	*	*	*	*	*	*	*	*	*	*	*	*	*
433	*		*		*		*		*		*		*
443	*	*	*	*	*	*	*	*	*	*	*	*	*
441	*	*	*	*	*	*	*	*	*	*	*	*	*

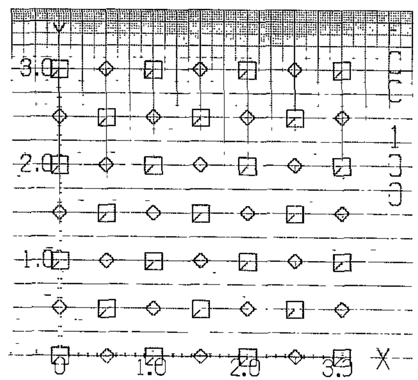
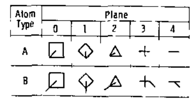


Figure 1. - Face-centered-cubic structure; 100 plane.



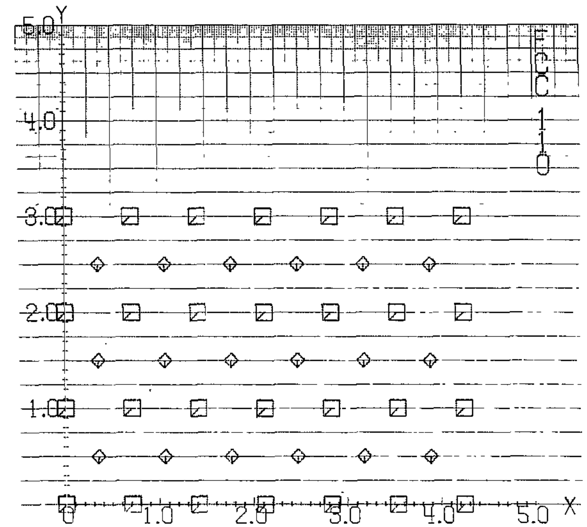


Figure 2. - Face-centered-cubic structure; 110 plane.

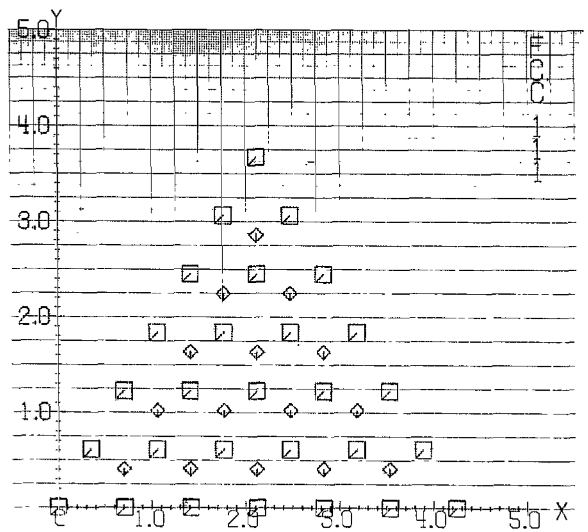


Figure 3. - Face-centered-cubic structure; 111 plane.

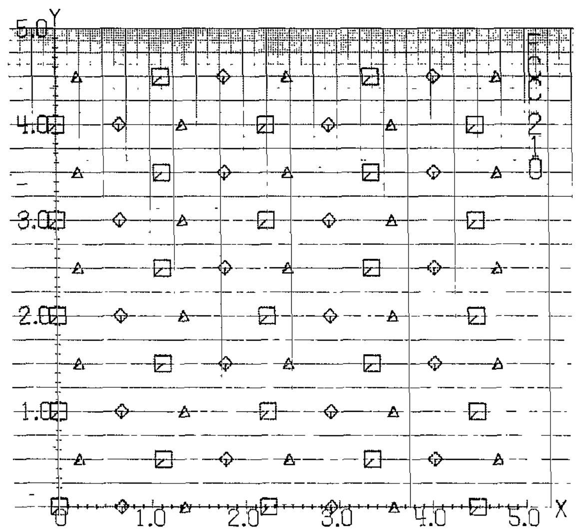


Figure 4. - Face-centered-cubic structure; 210 plane.

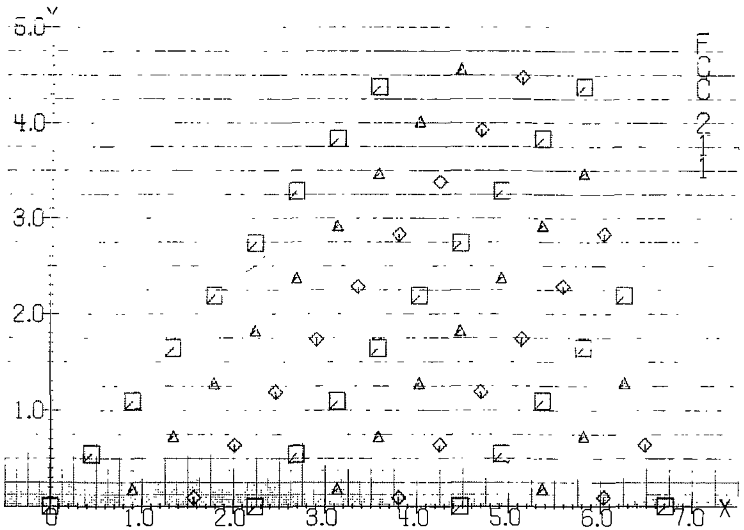
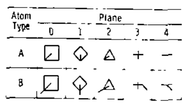


Figure 5. - Face-centered-cubic structure; 211 plane.



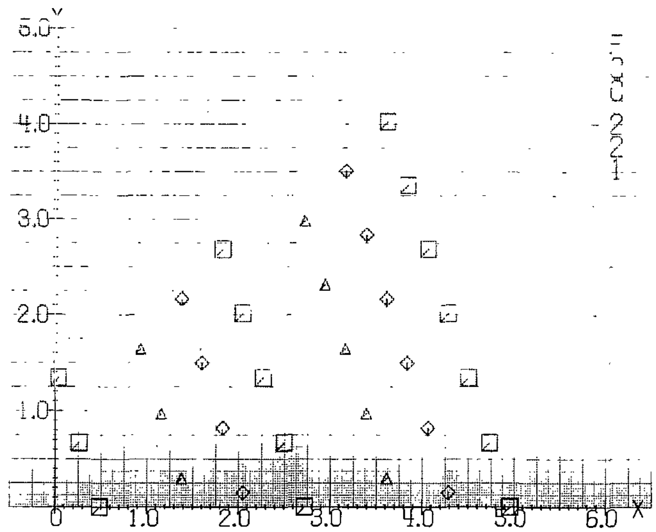


Figure 6. - Face-centered-cubic structure; 221 plane.

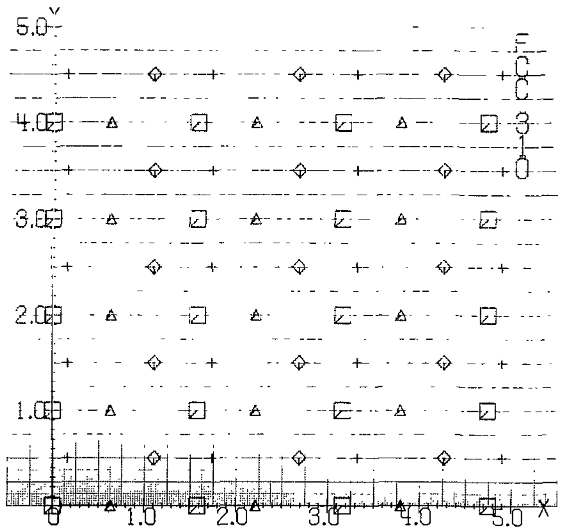


Figure 7. - Face-centered-cubic structure; 310 plane.

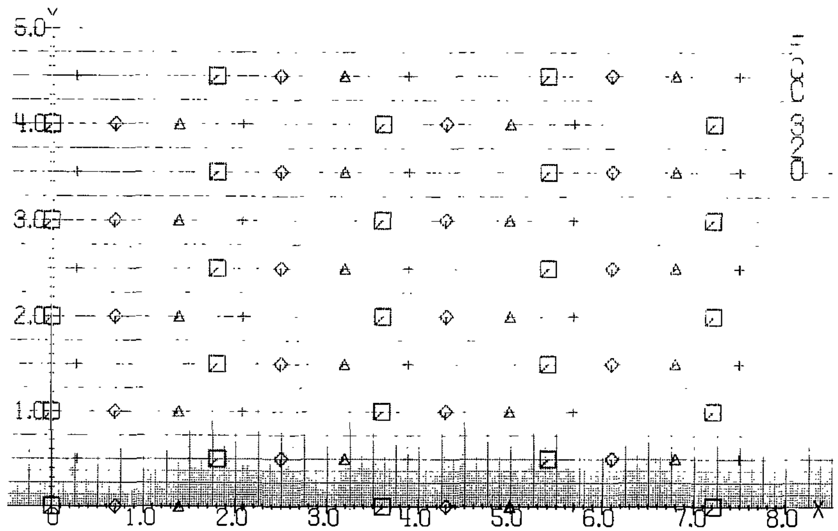


Figure 8. - Face-centered-cubic structure; 320 plane.

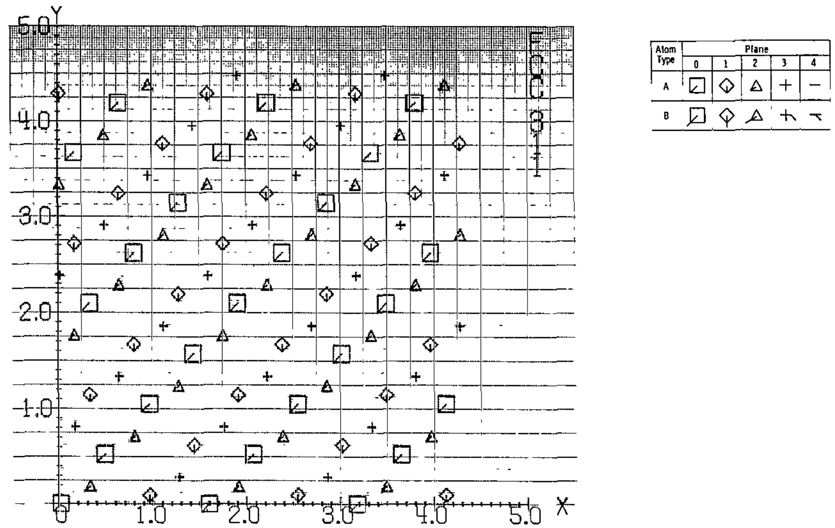


Figure 9. - Face-centered-cubic structure; 311 plane.

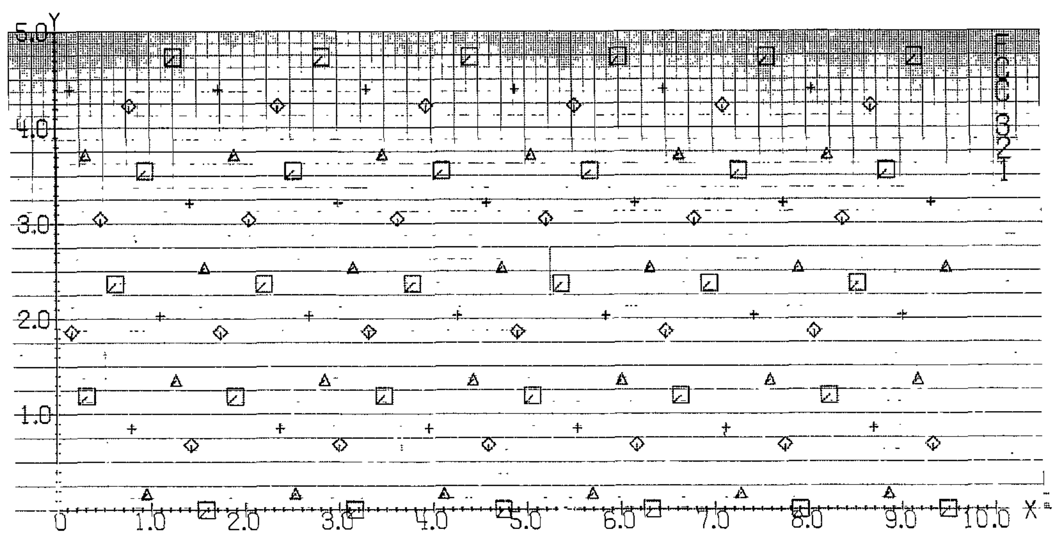


Figure 10. - Face-centered-cubic structure; 321 plane.

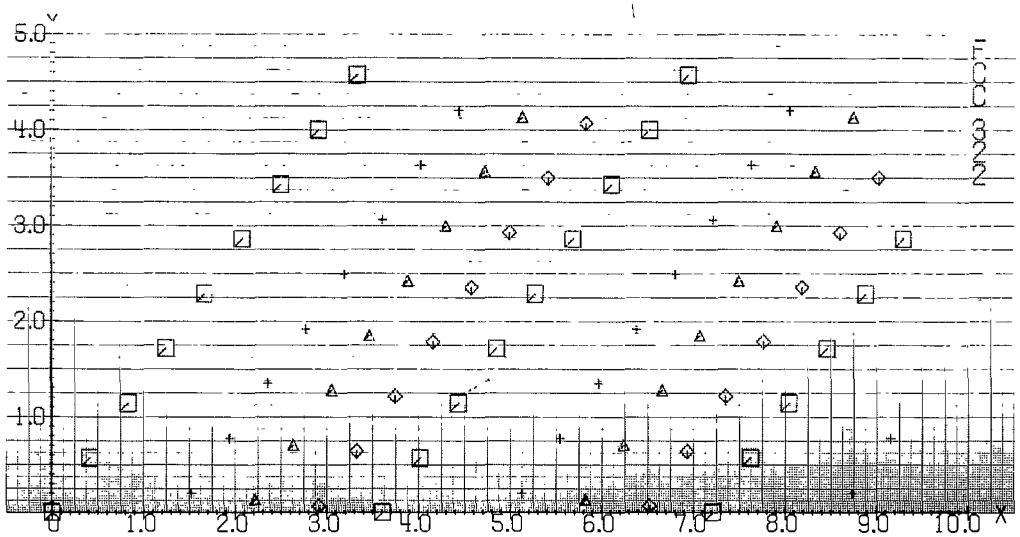


Figure 11. - Face-centered-cubic structure; 322 plane.

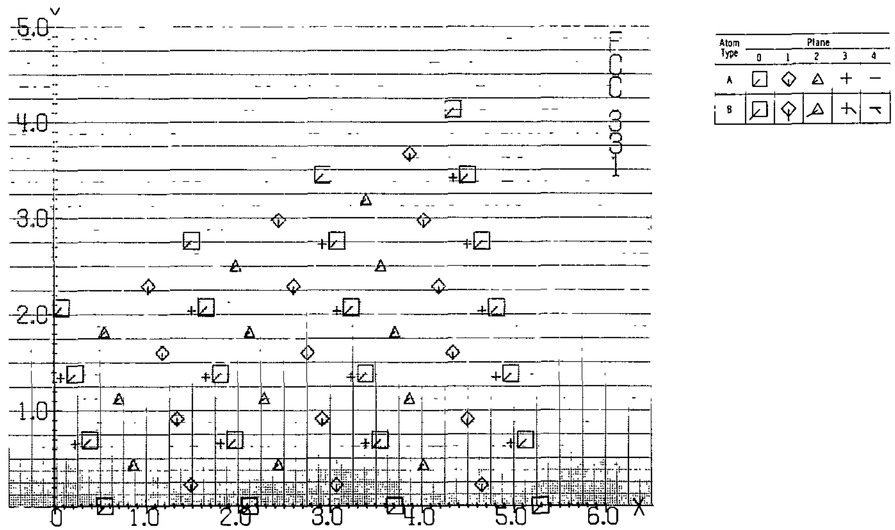


Figure 12. - Face-centered-cubic structure; 331 plane.

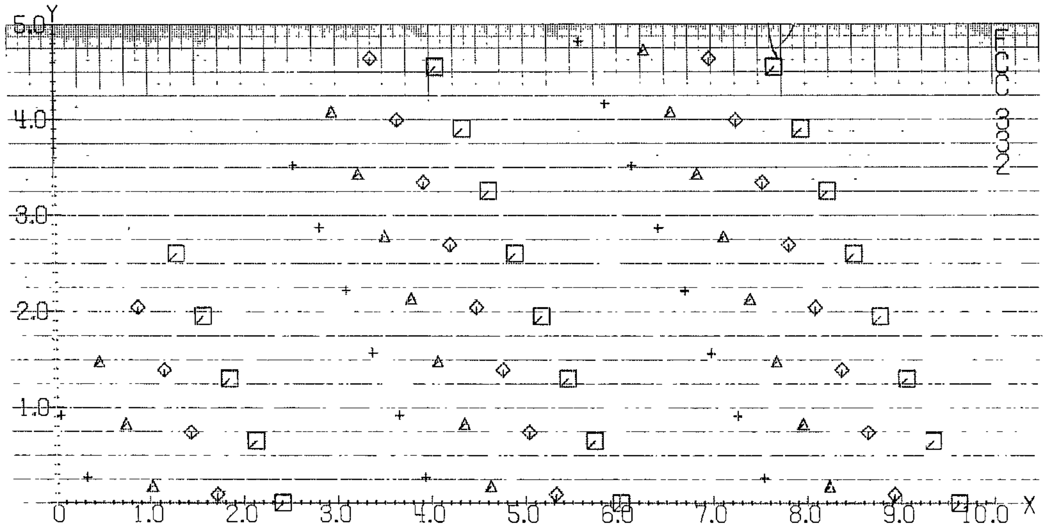
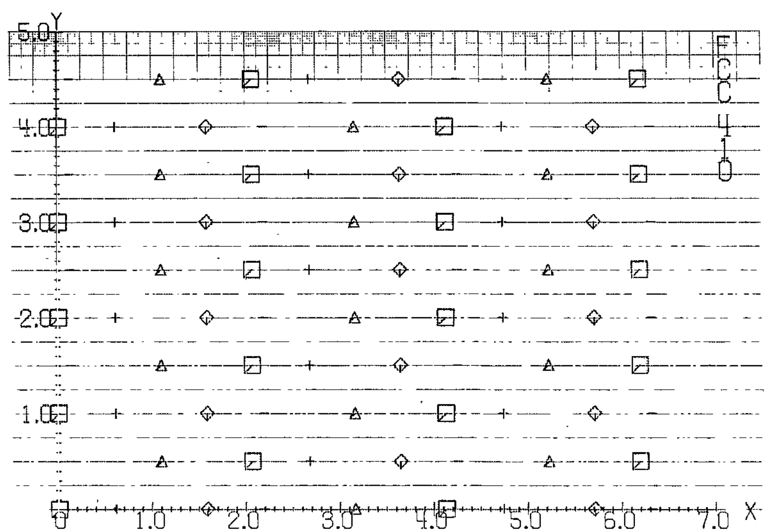


Figure 13. - Face-centered-cubic structure; 332 plane.



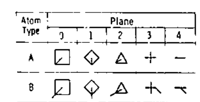


Figure 14. - Face-centered-cubic structure; 410 plane.

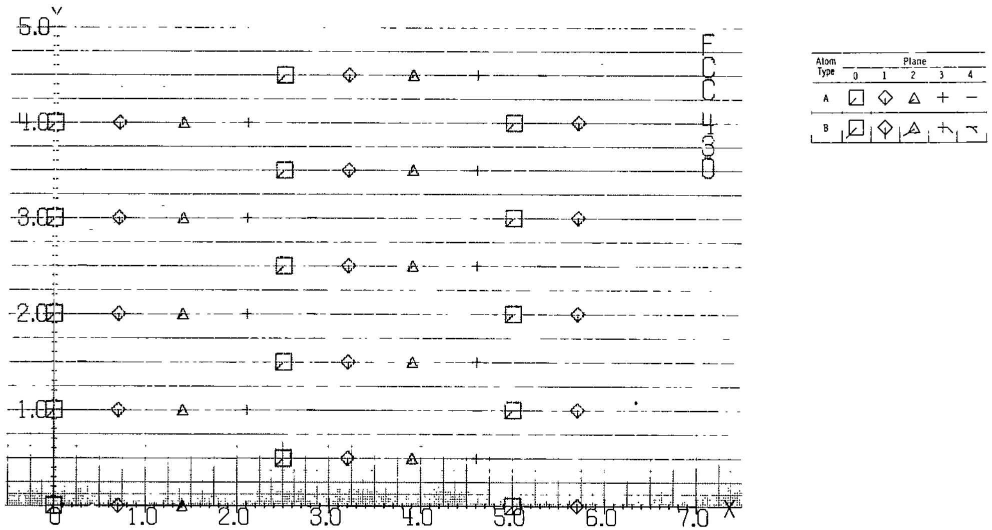


Figure 15. - Face-centered-cubic structure; 430 plane.

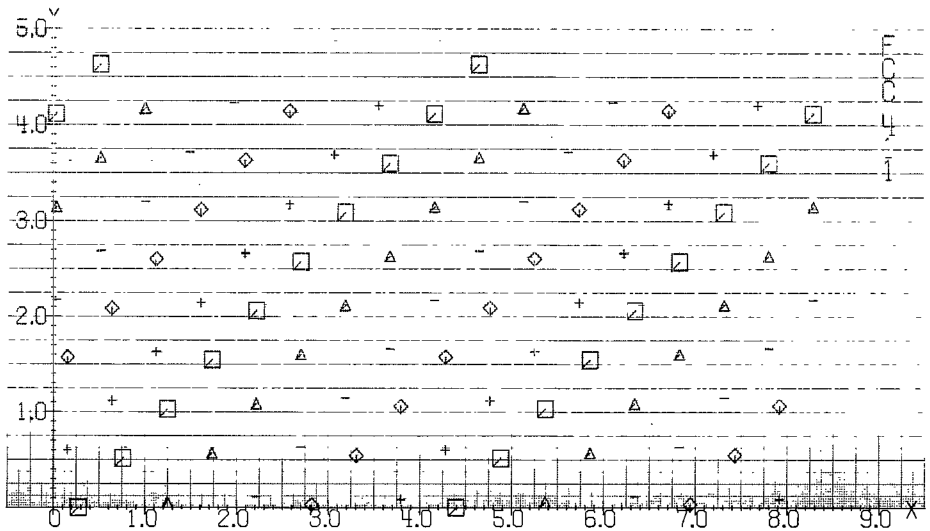


Figure 16. - Face-centered-cubic structure; 411 plane.

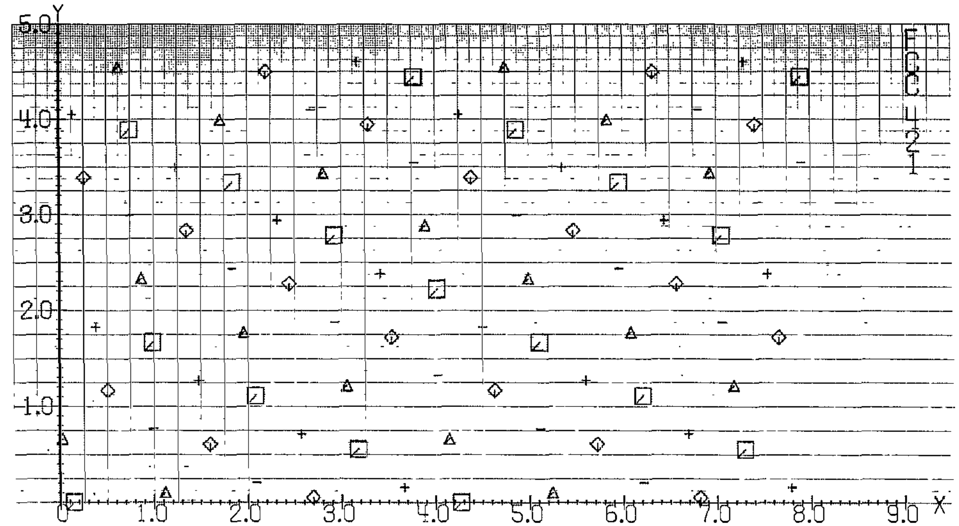
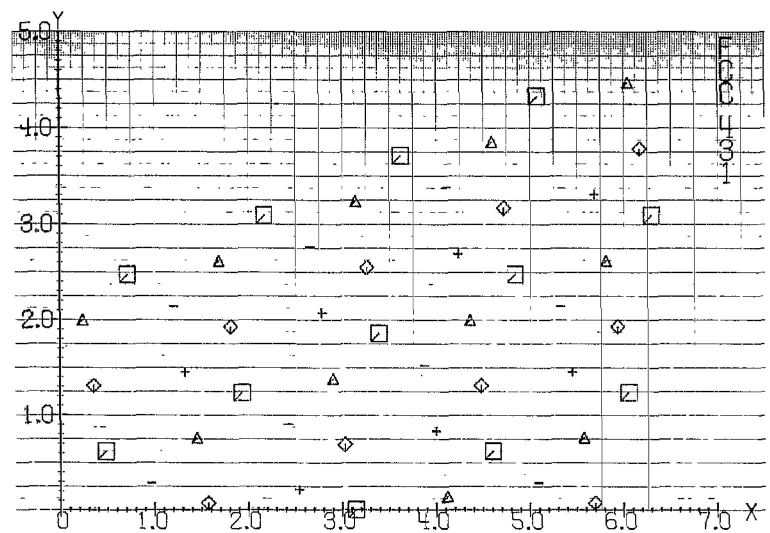


Figure 17. - Face-centered-cubic structure; 421 plane.



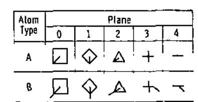


Figure 18. - Face-centered-cubic structure; 431 plane.

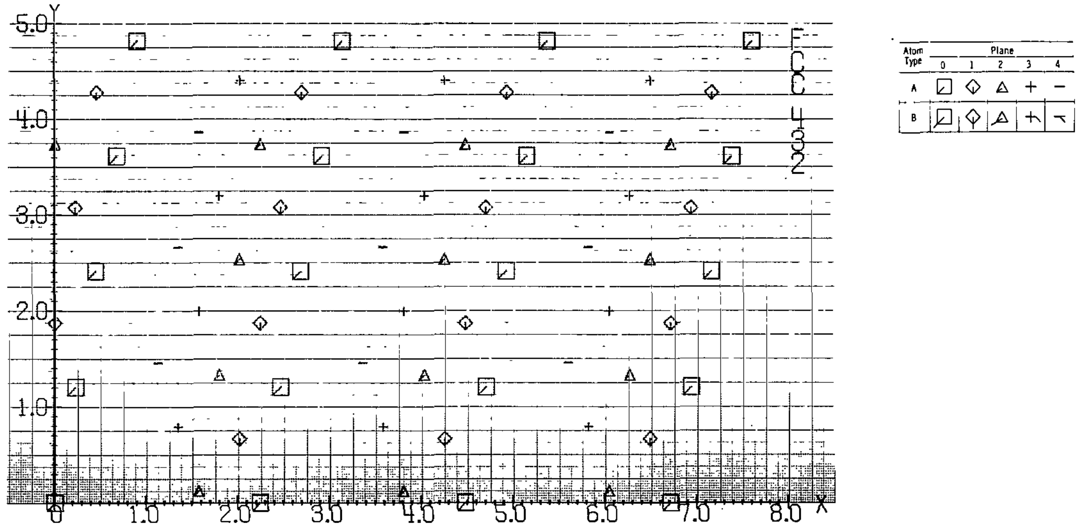


Figure 19. - Face-centered-cubic structure; 432 plane.

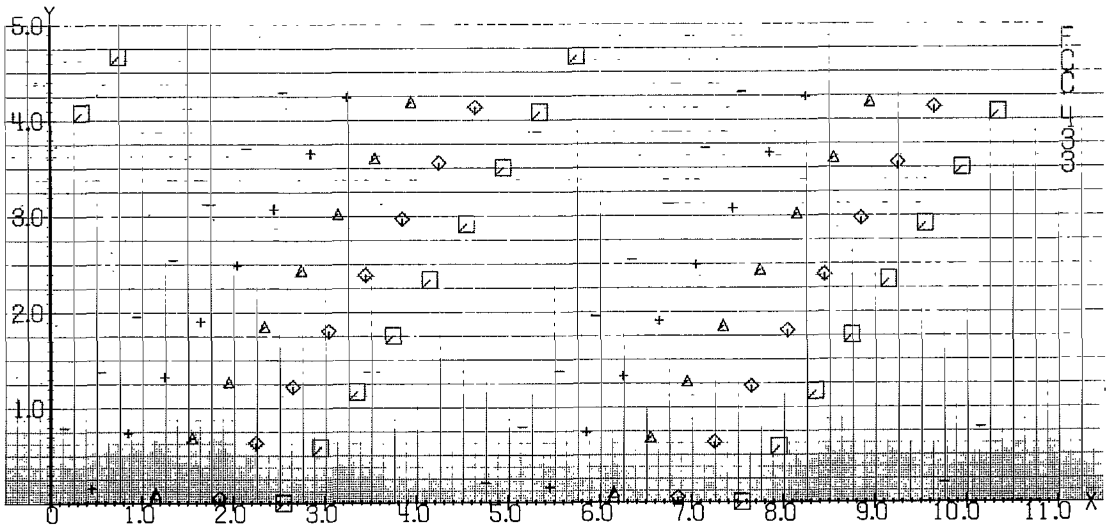


Figure 20. - Face-centered-cubic structure; 433 plane.

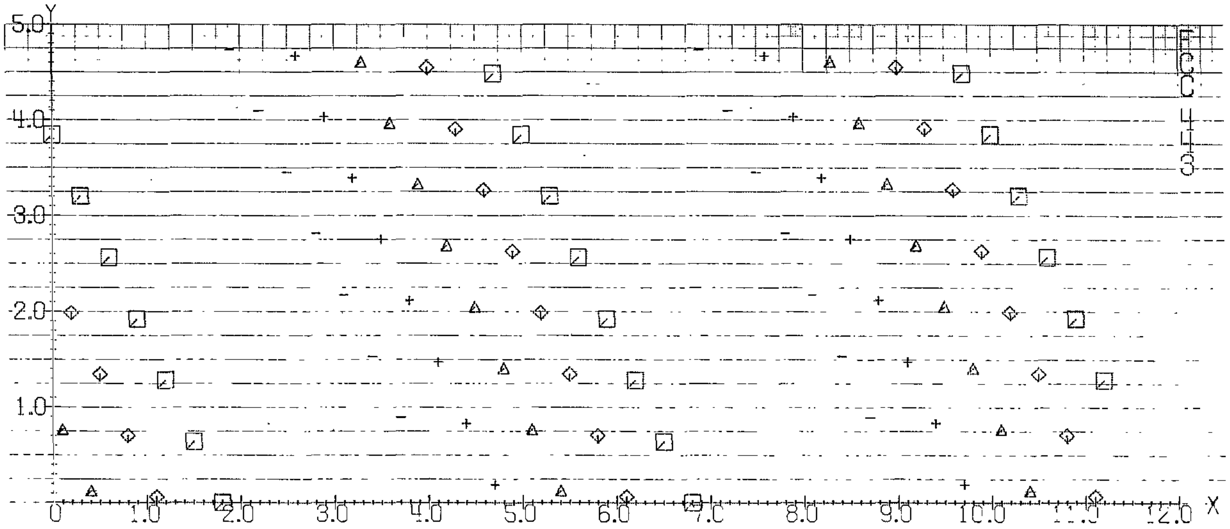
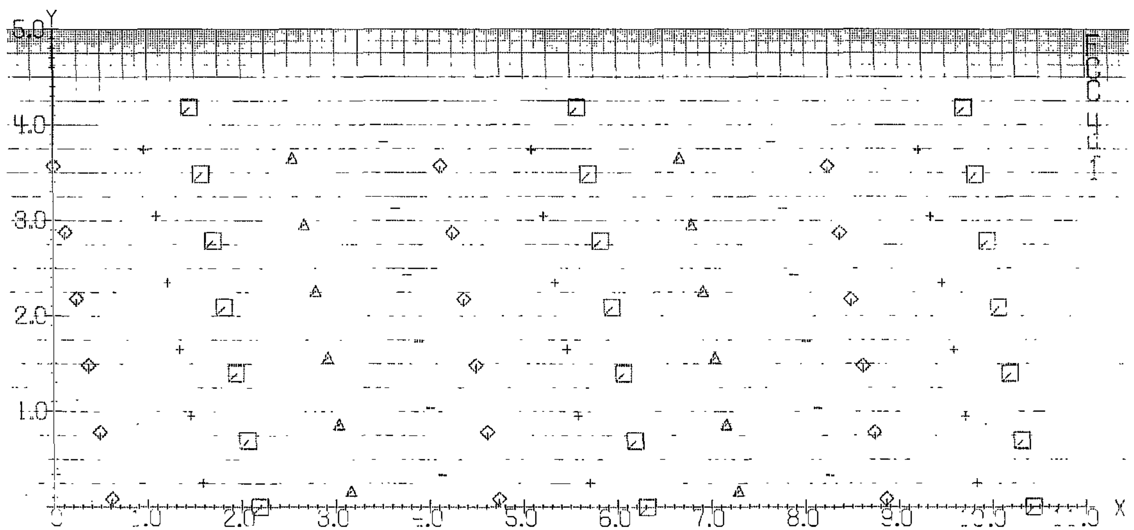


Figure 21. - Face-centered-cubic structure; 443 plane.



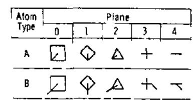


Figure 22. - Face-centered-cubic structure; 441 plane.

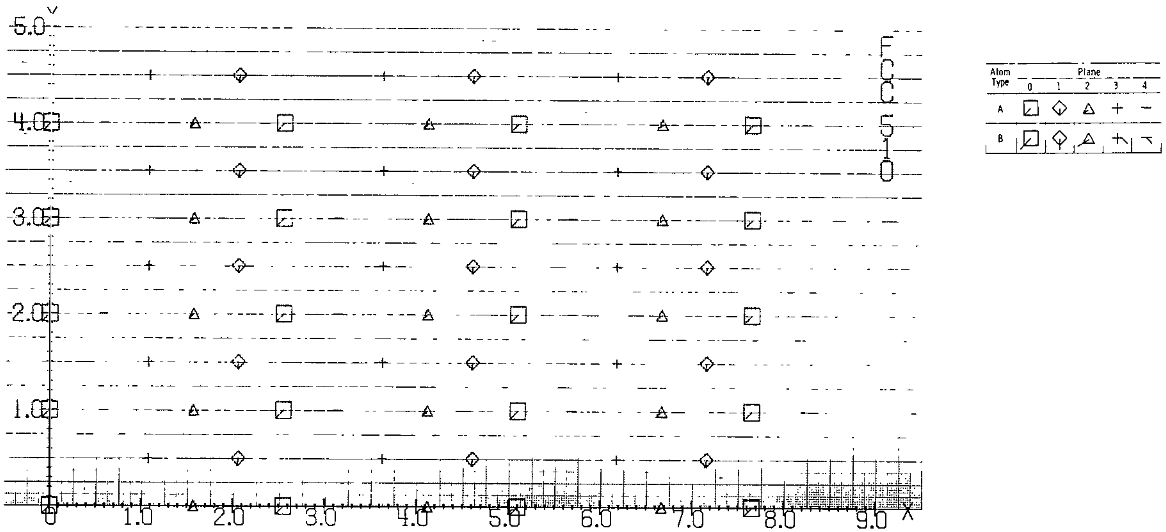


Figure 23. - Face-centered-cubic structure; 510 plane.

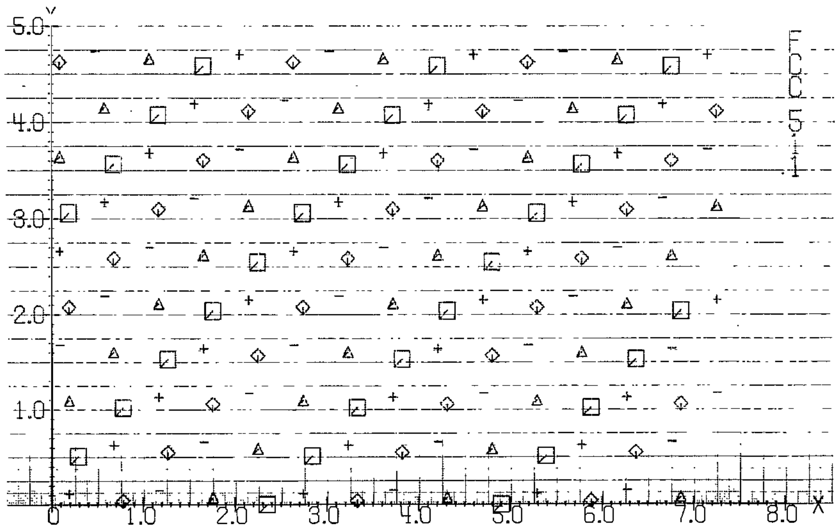


Figure 24. - Face-centered-cubic structure; 511 plane.

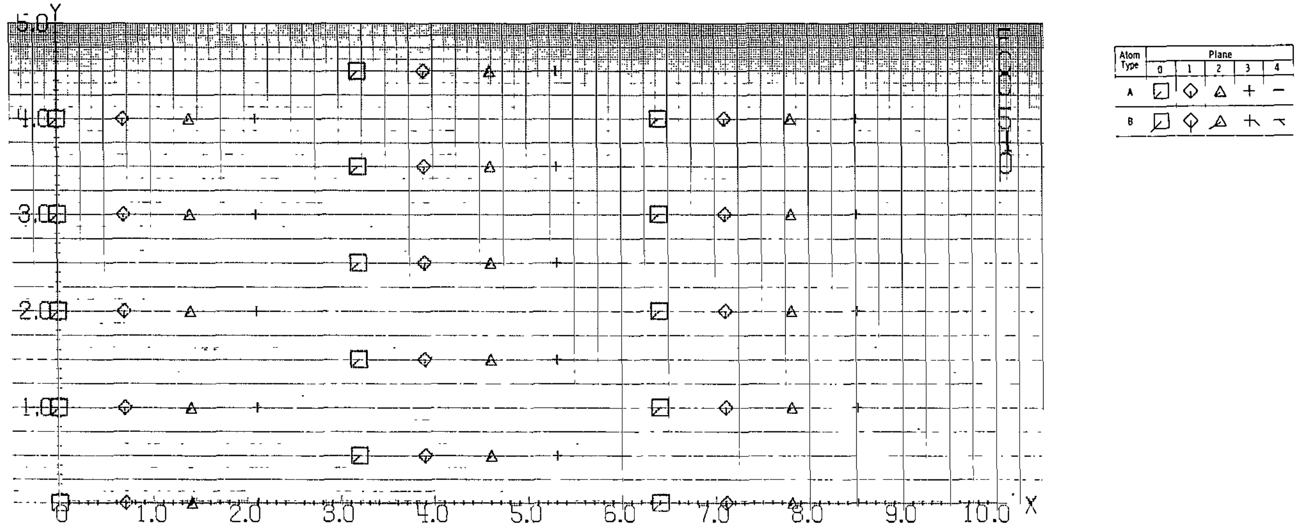


Figure 25. - Face-centered-cubic structure; 540 plane.

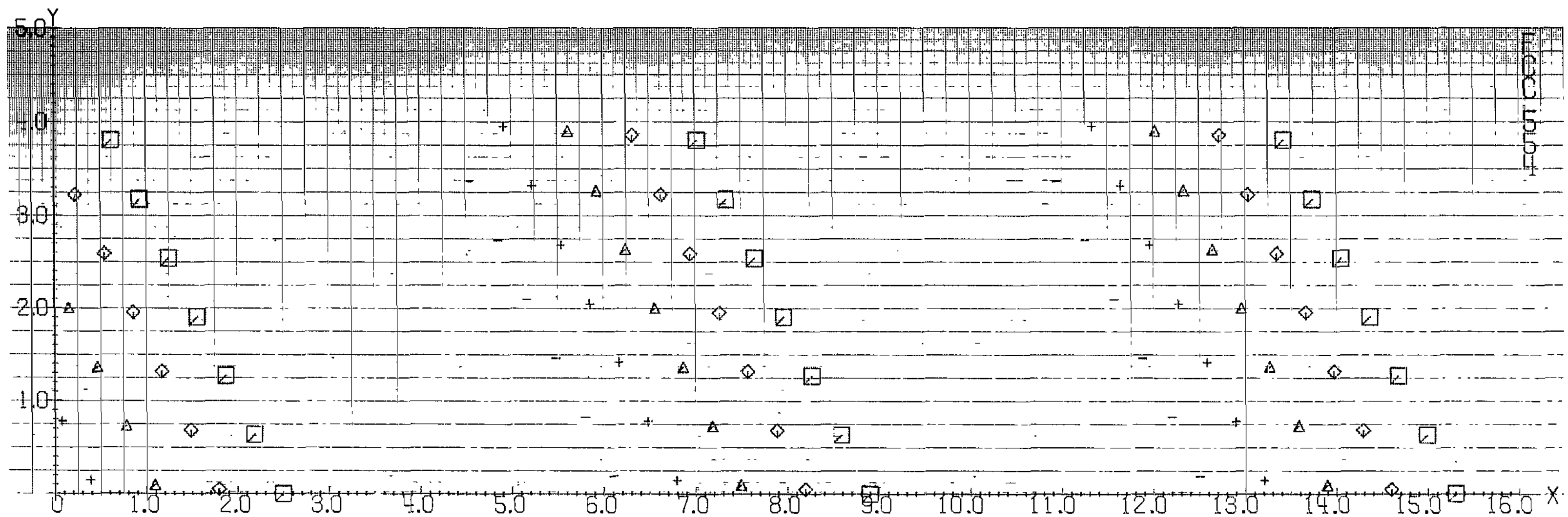
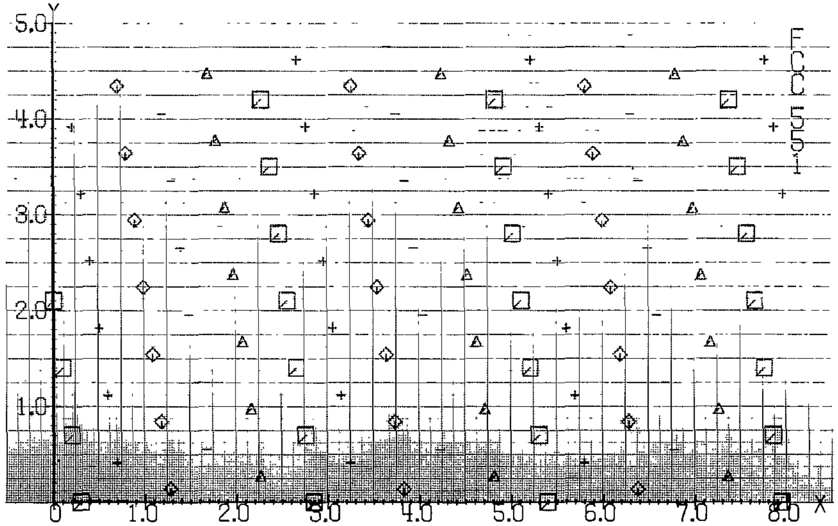


Figure 26. - Face-centered-cubic structure; 554 plane.



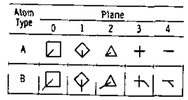


Figure 27. - Face-centered-cubic structure; 551 plane.

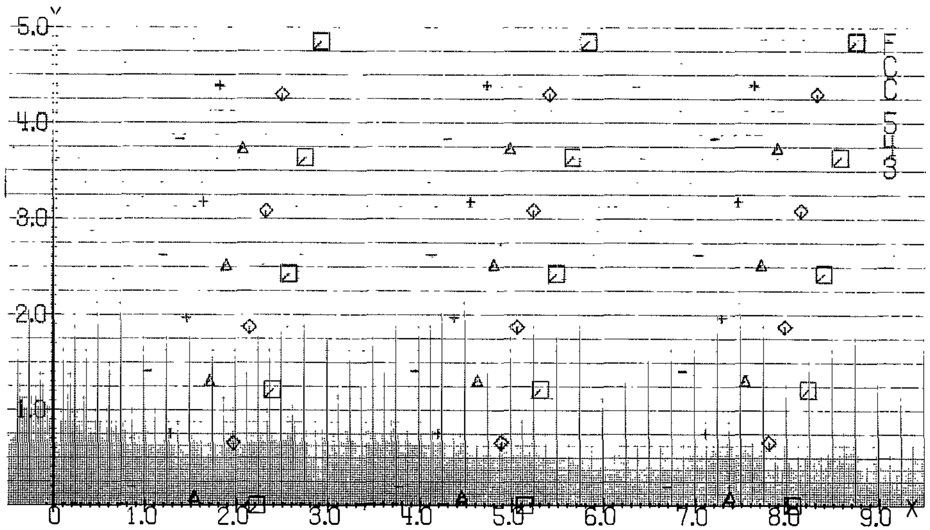


Figure 28. - Face-centered-cubic structure; 543 plane.

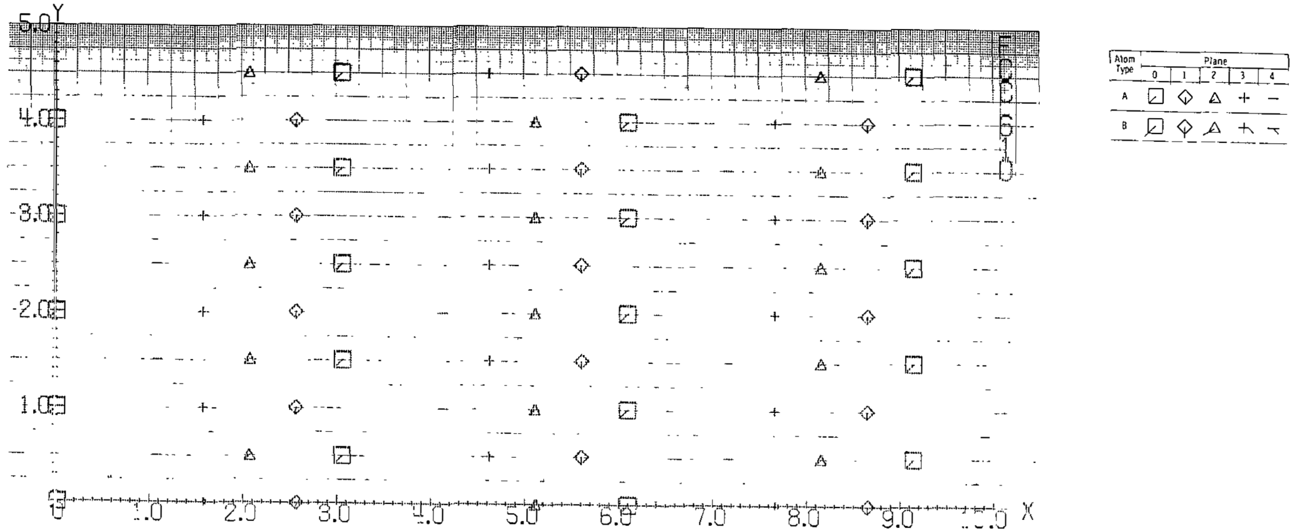


Figure 29. - Face-centered-cubic structure; 610 plane.

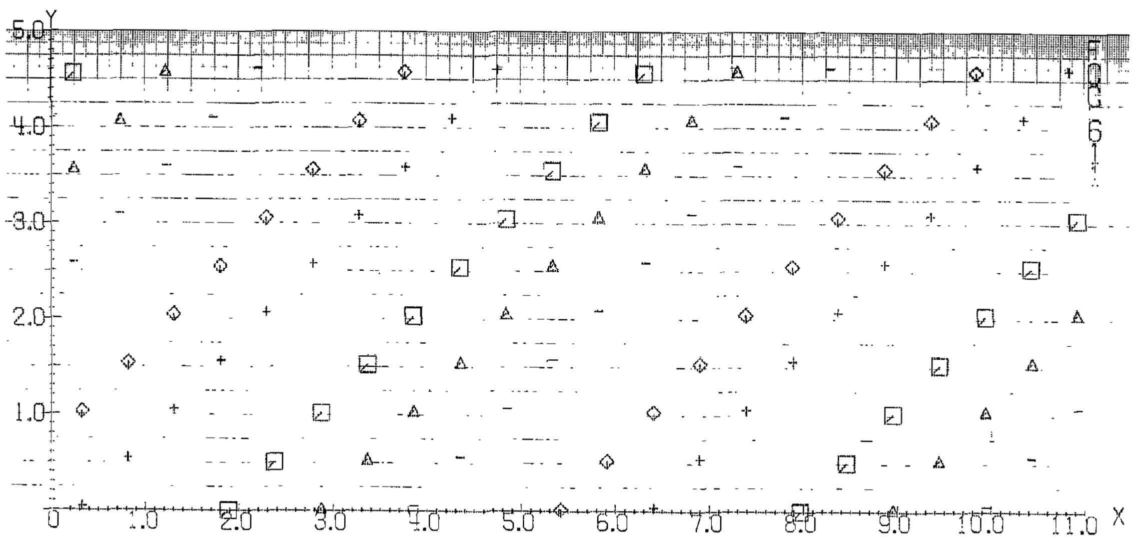


Figure 30. - Face-centered-cubic structure; 611 plane.

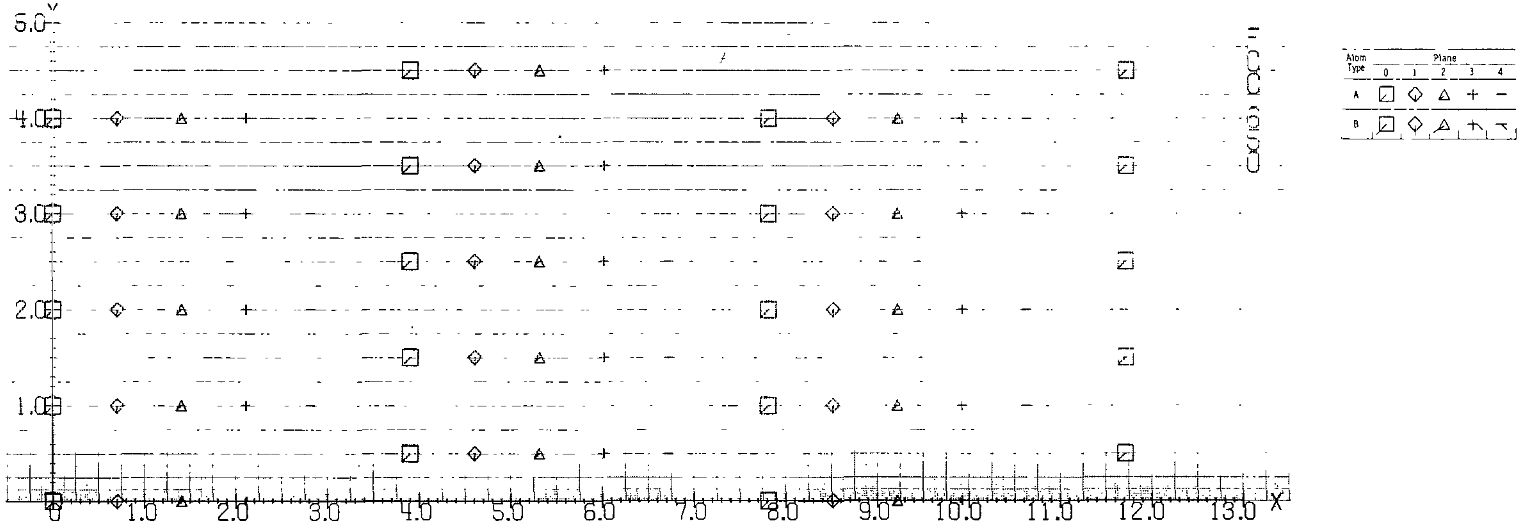


Figure 31. - Face-centered-cubic structure; 650 plane.

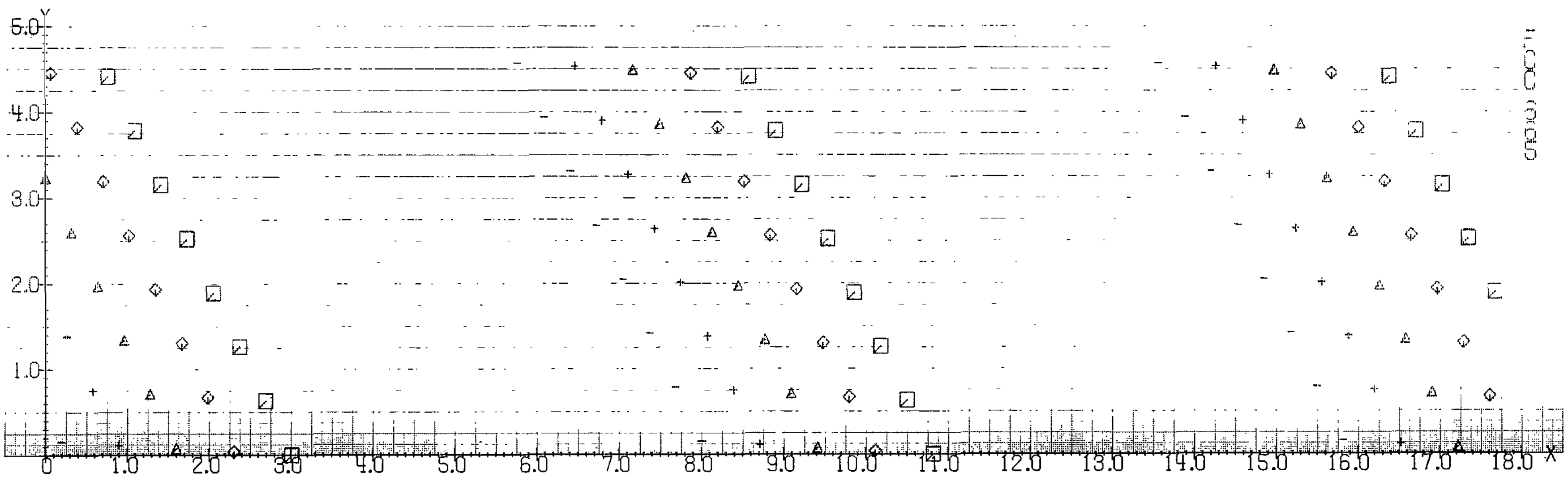


Figure 32. - Face-centered-cubic structure; 665 plane.

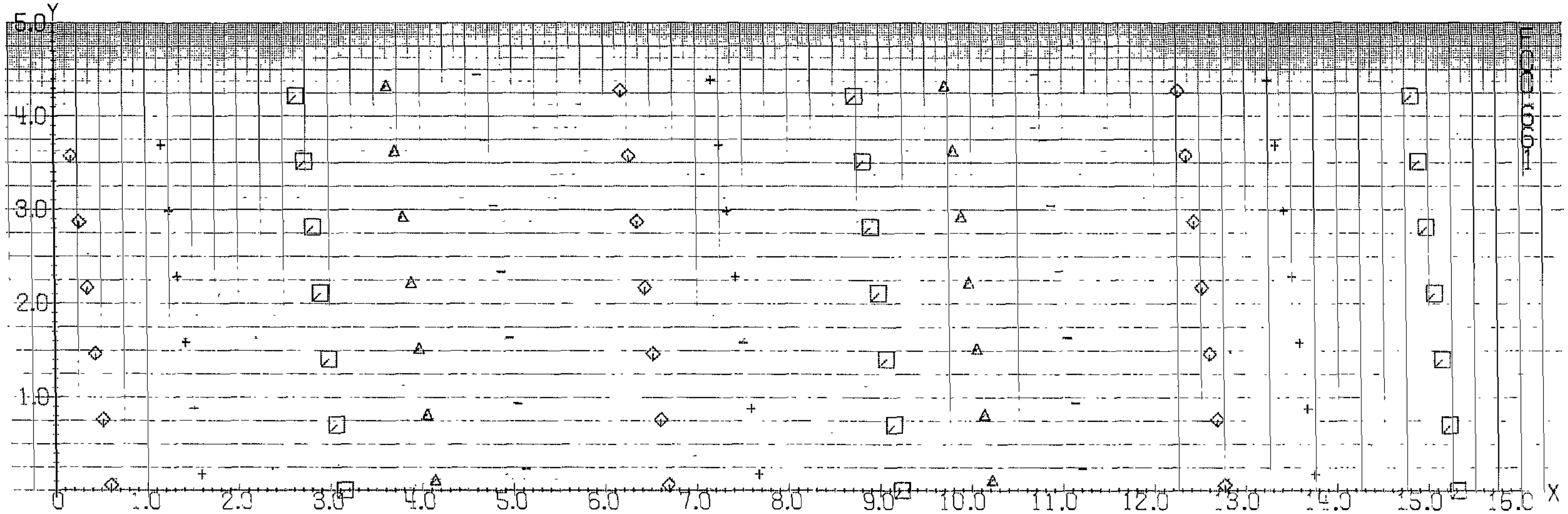
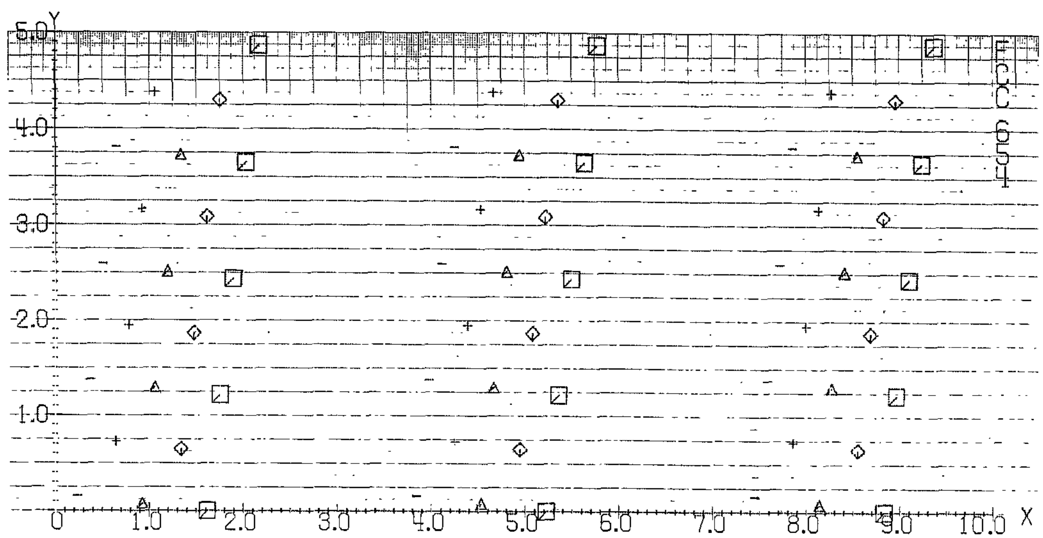


Figure 33. - Face-centered-cubic structure; 661 plane.



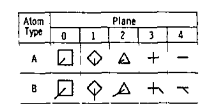


Figure 34. - Face-centered-cubic structure; 654 plane.

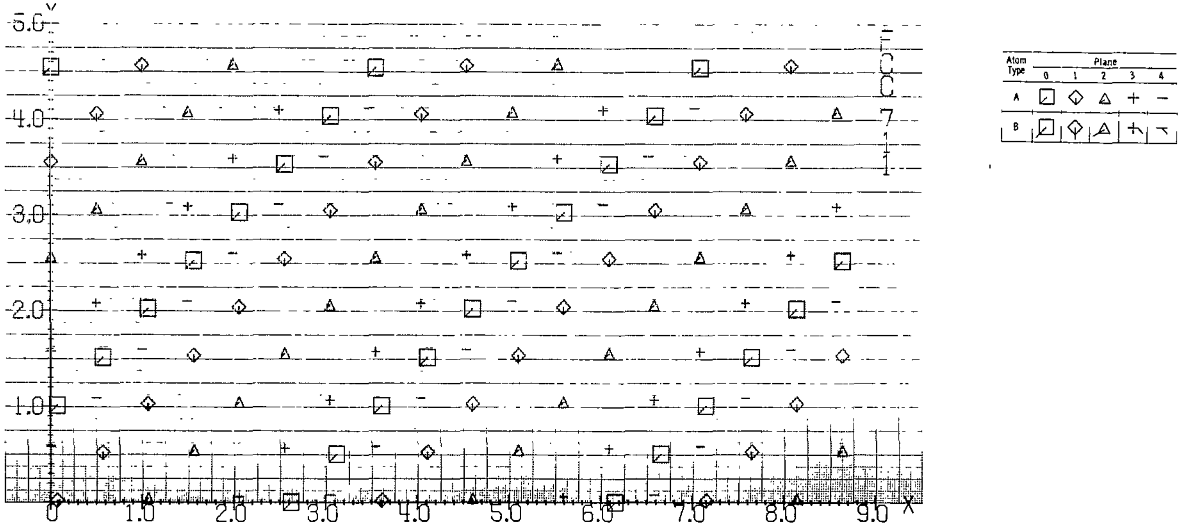


Figure 35. - Face-centered-cubic structure; 711 plane.

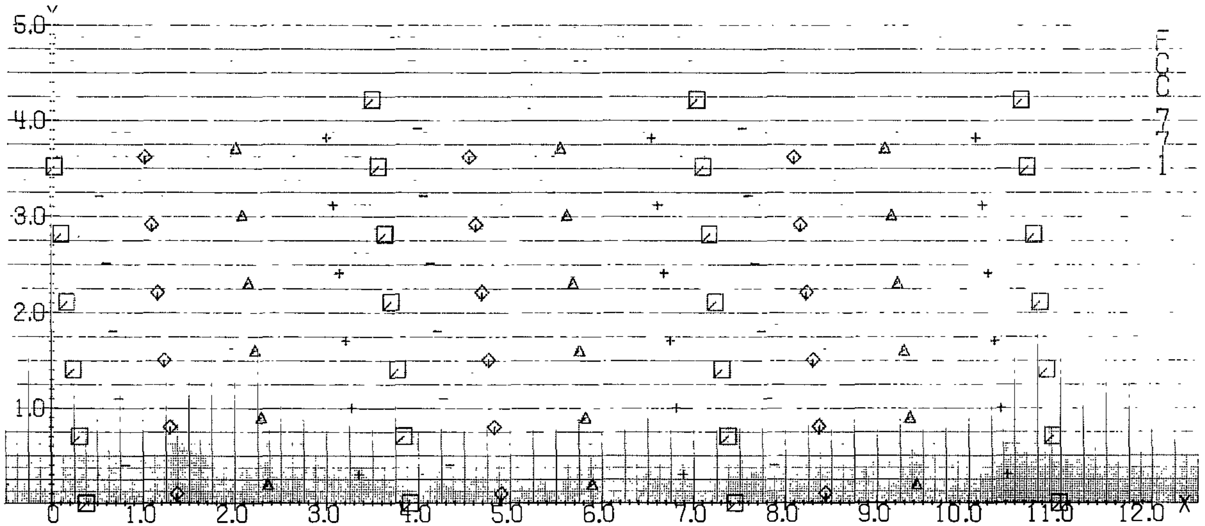


Figure 36. - Face-centered-cubic structure; 771 plane.

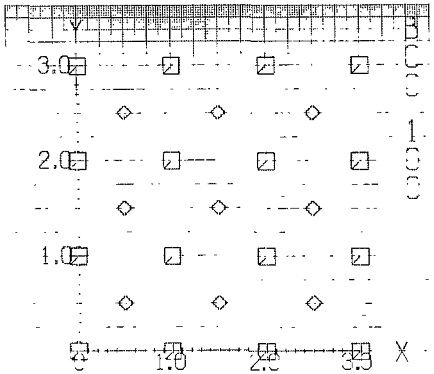


Figure 37. - Body-centered-cubic structure; 100 plane.

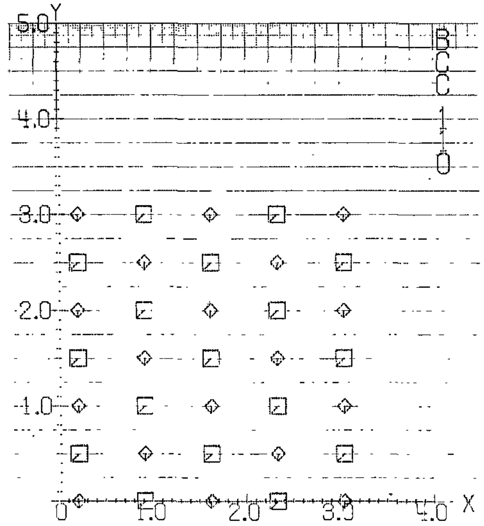


Figure 38. - Body-centered-cubic structure; 110 plane.

Atom Type	Plane 0	1	2	3	4
A	◻	◇	△	+	−
B	◻	◇	△	+	−

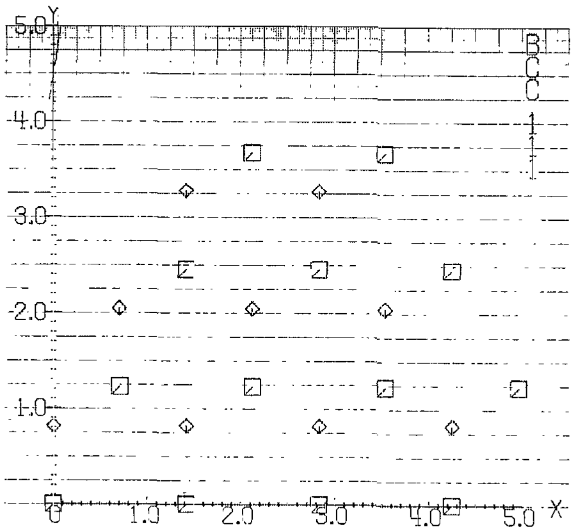


Figure 39. - Body-centered-cubic structure; 111 plane.

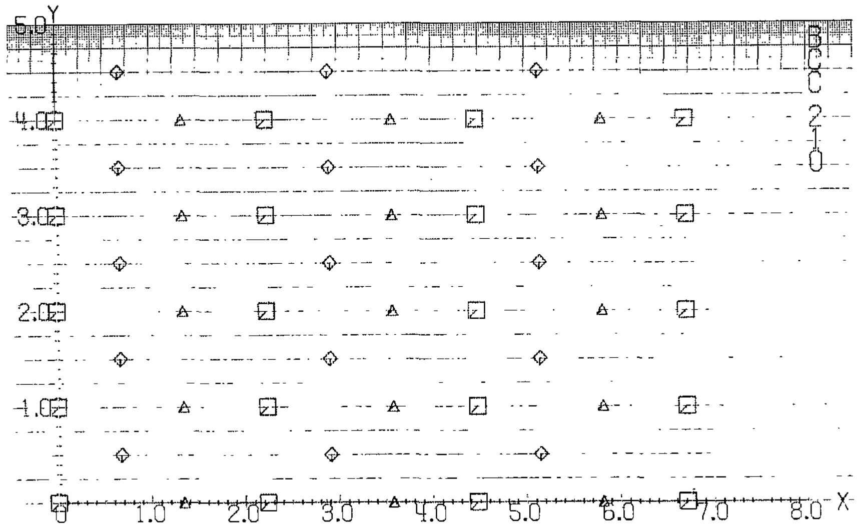


Figure 40. - Body-centered-cubic structure; 210 plane.

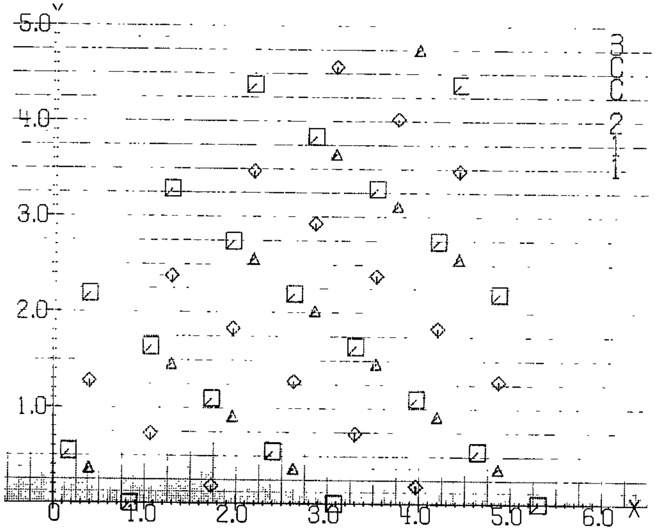


Figure 41. - Body-centered-cubic structure; 211 plane.

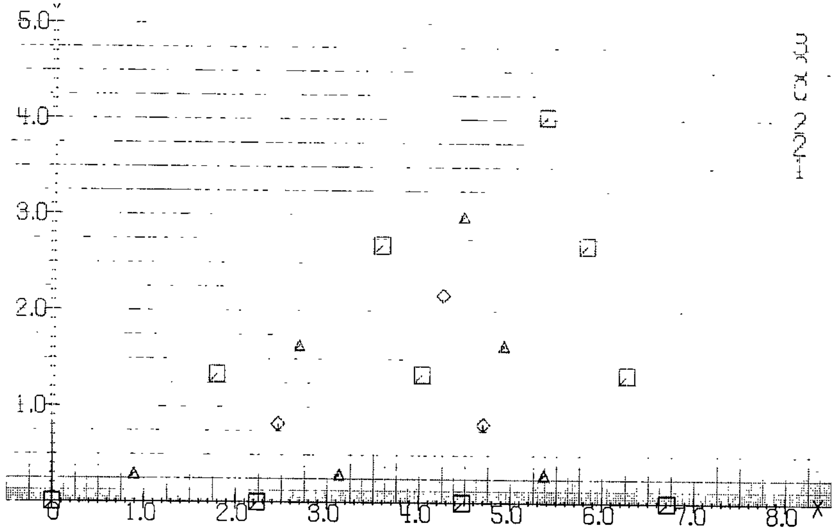
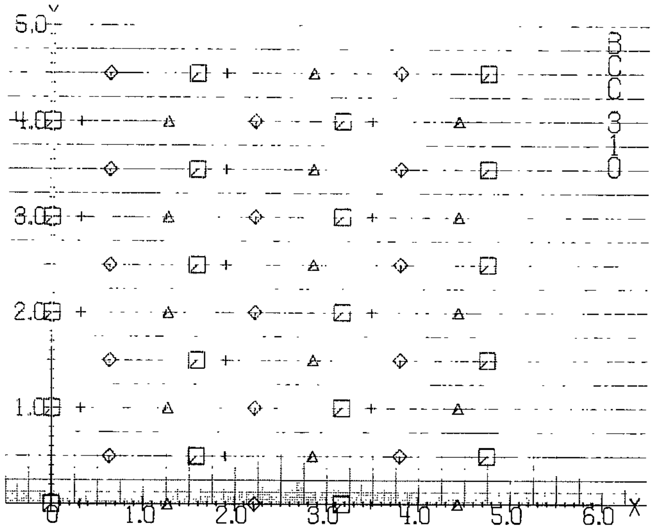


Figure 42. - Body-centered-cubic structure; 221 plane.



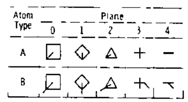


Figure 43. - Body-centered-cubic structure; 310 plane.

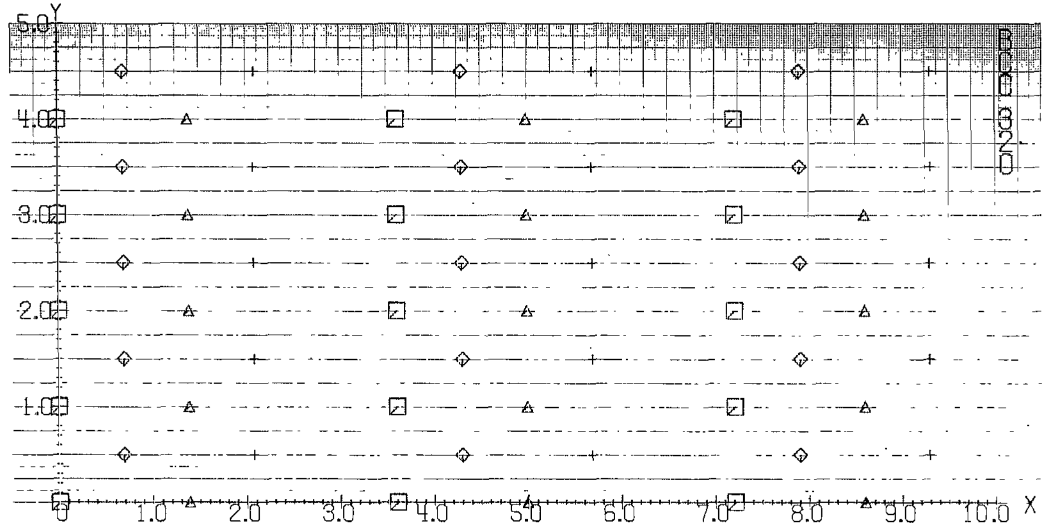


Figure 44. - Body-centered-cubic structure; 320 plane.

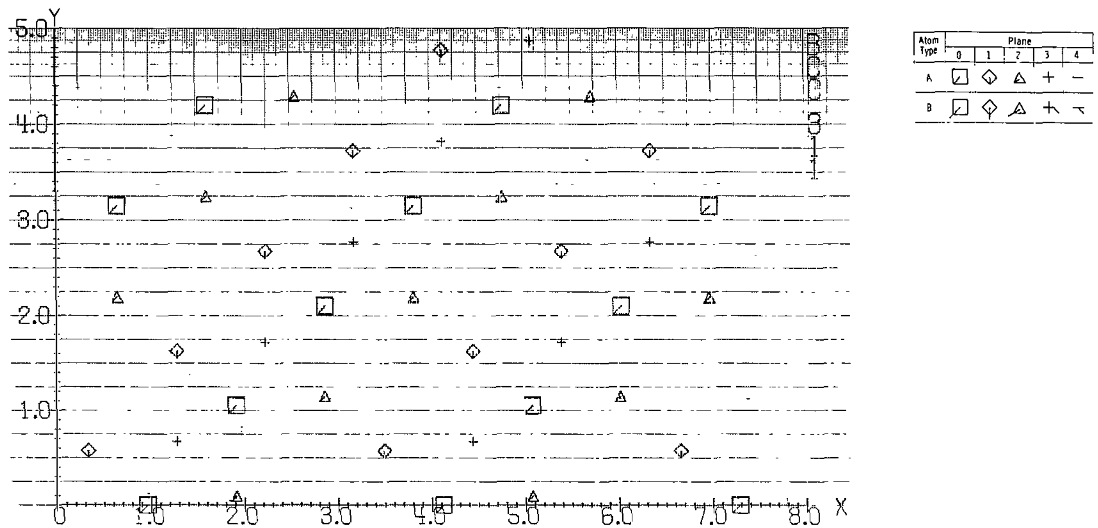
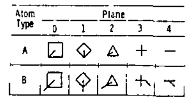


Figure 45. - Body-centered-cubic structure; 311 plane.



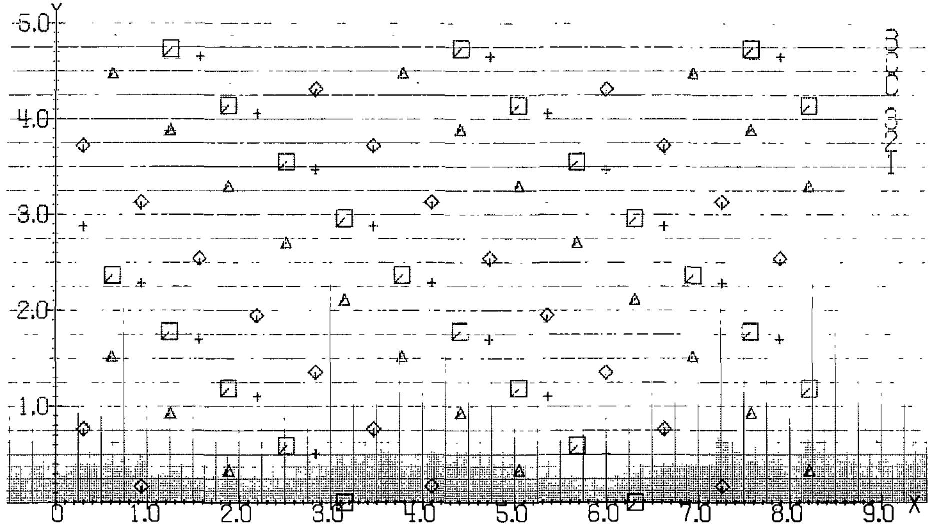


Figure 46. - Body-centered-cubic structure; 321 plane.

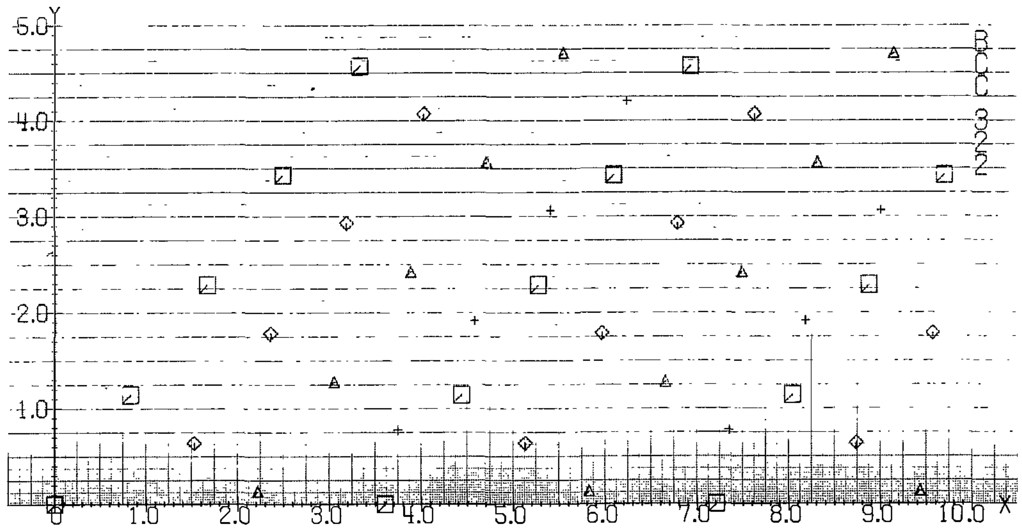


Figure 47. - Body-centered-cubic structure; 322 plane.

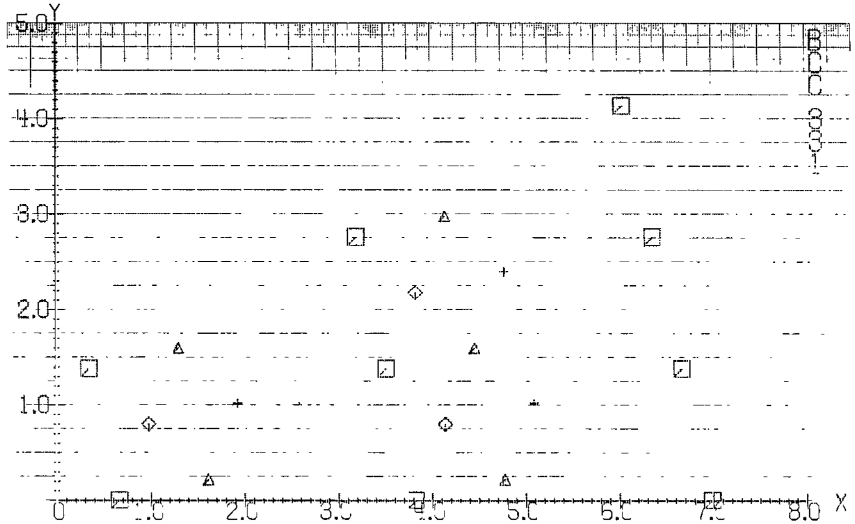
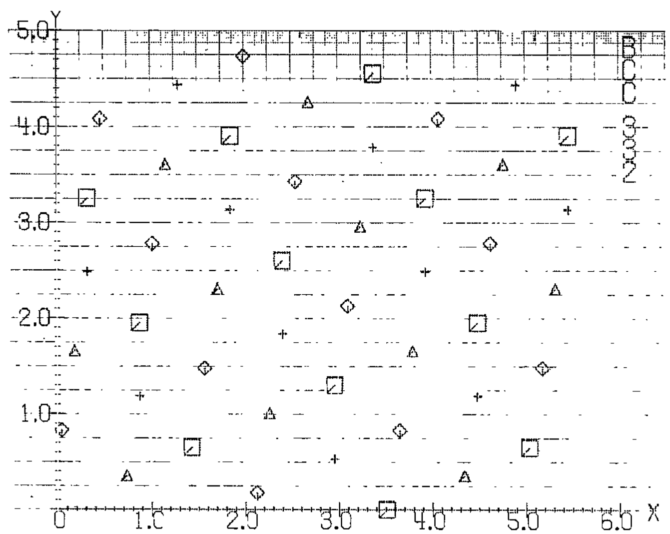


Figure 48. - Body-centered-cubic structure; 331 plane.



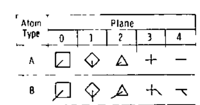


Figure 49. - Body-centered-cubic structure; 332 plane.

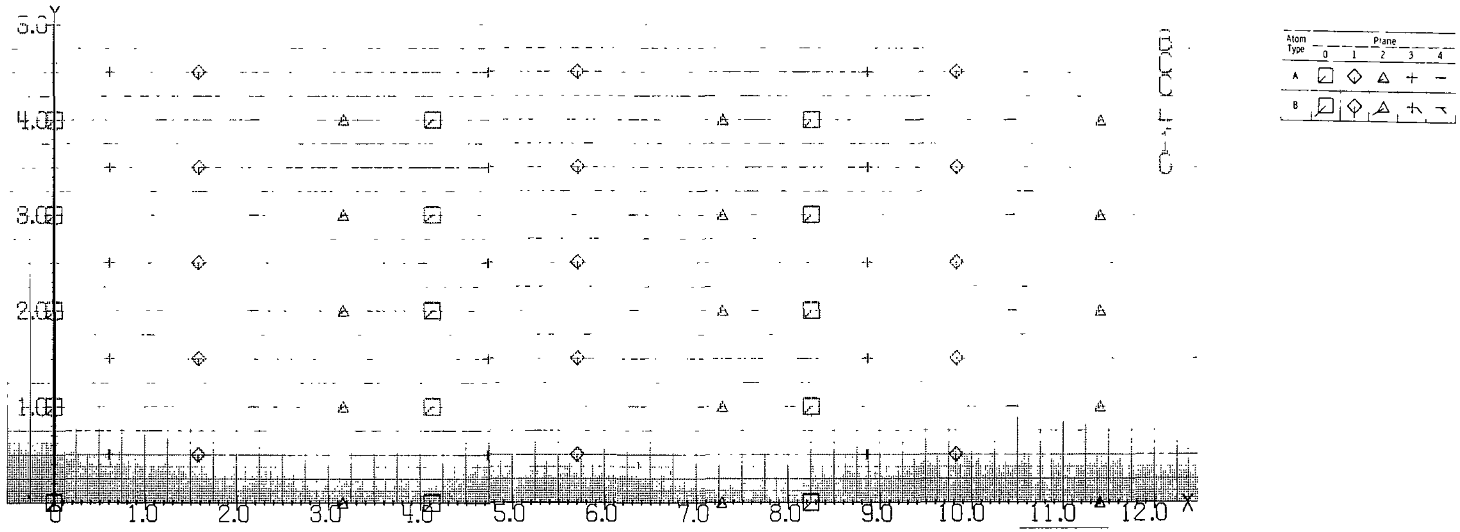


Figure 50. - Body-centered-cubic structure; 410 plane.

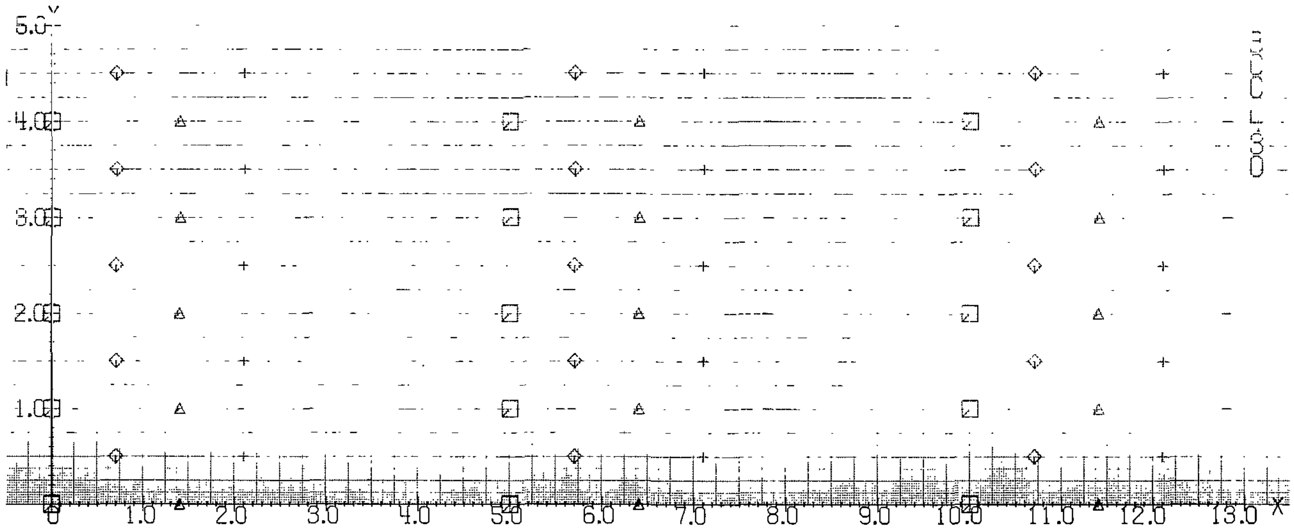
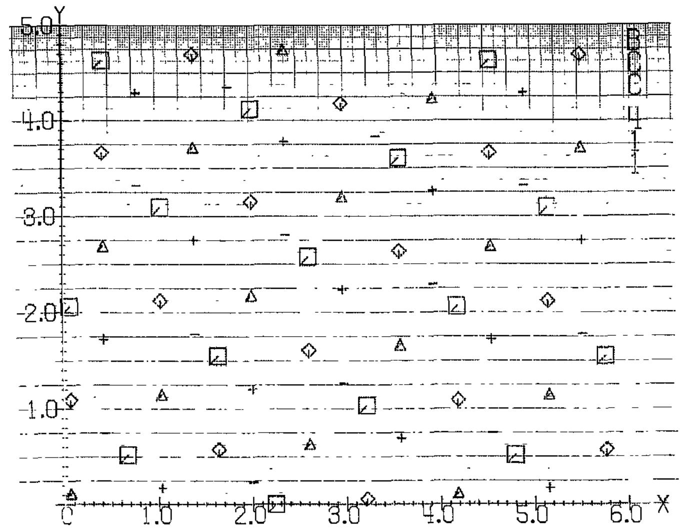


Figure 51. - Body-centered-cubic structure; 430 plane.



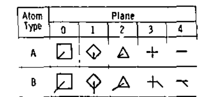


Figure 52. - Body-centered-cubic structure; 411 plane.

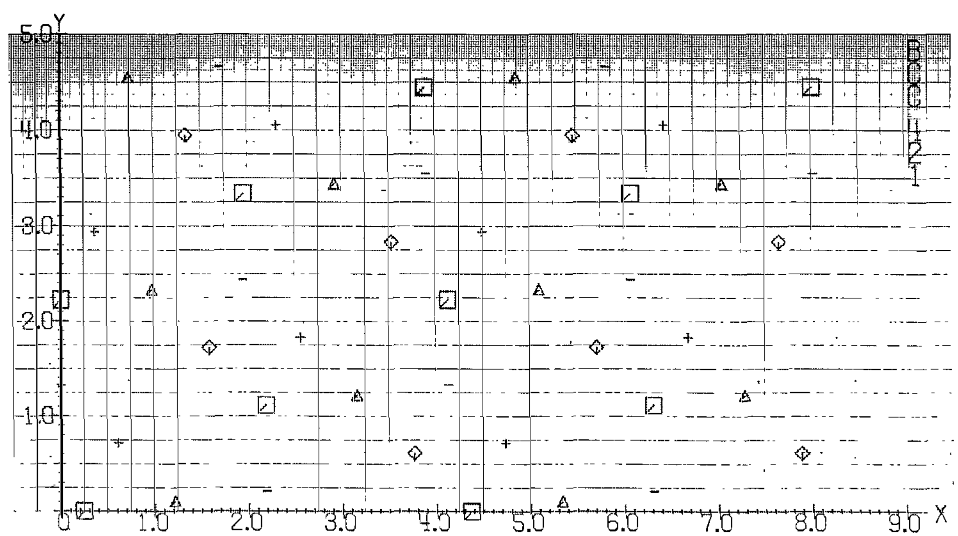
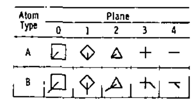


Figure 53. - Body-centered-cubic structure; 421 plane.



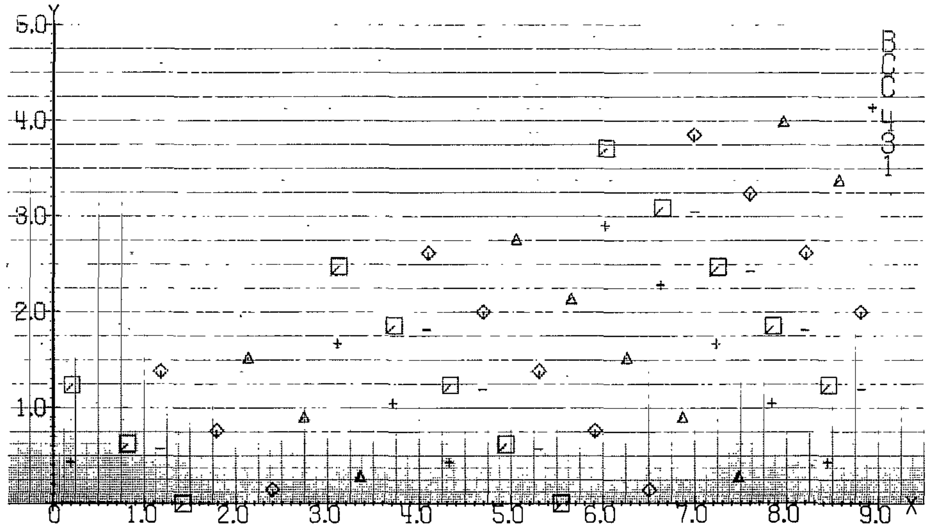


Figure 54. - Body-centered-cubic structure; 431 plane.

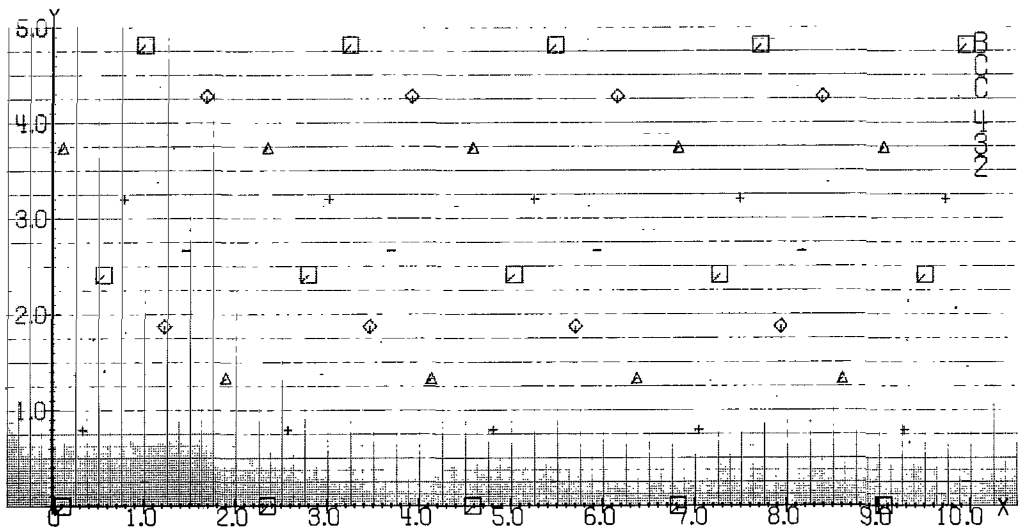


Figure 55. - Body-centered-cubic structure; 432 plane.

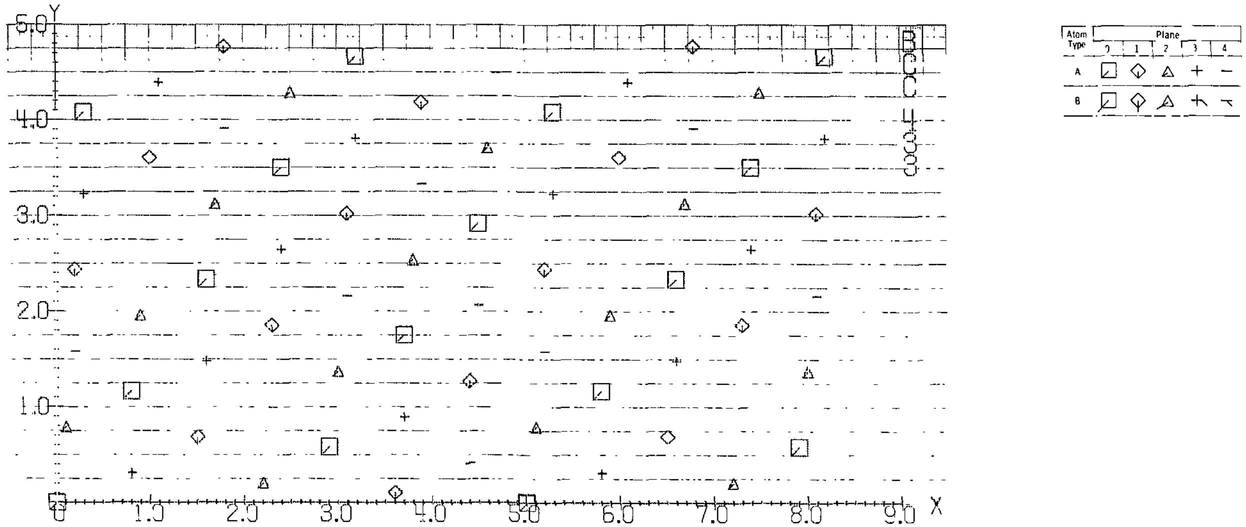


Figure 56. - Body-centered-cubic structure; 433 plane.

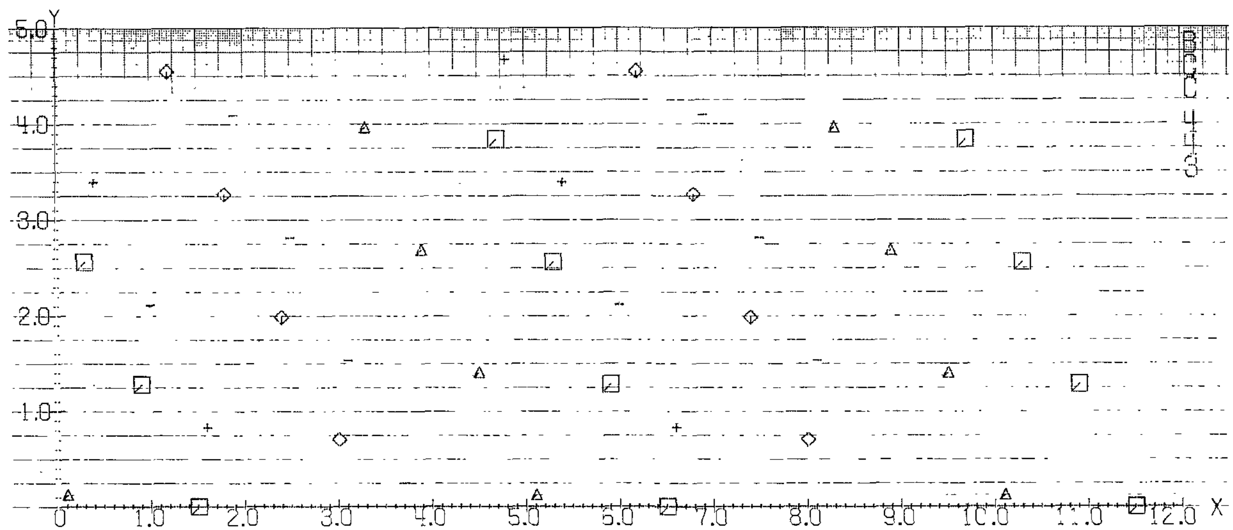
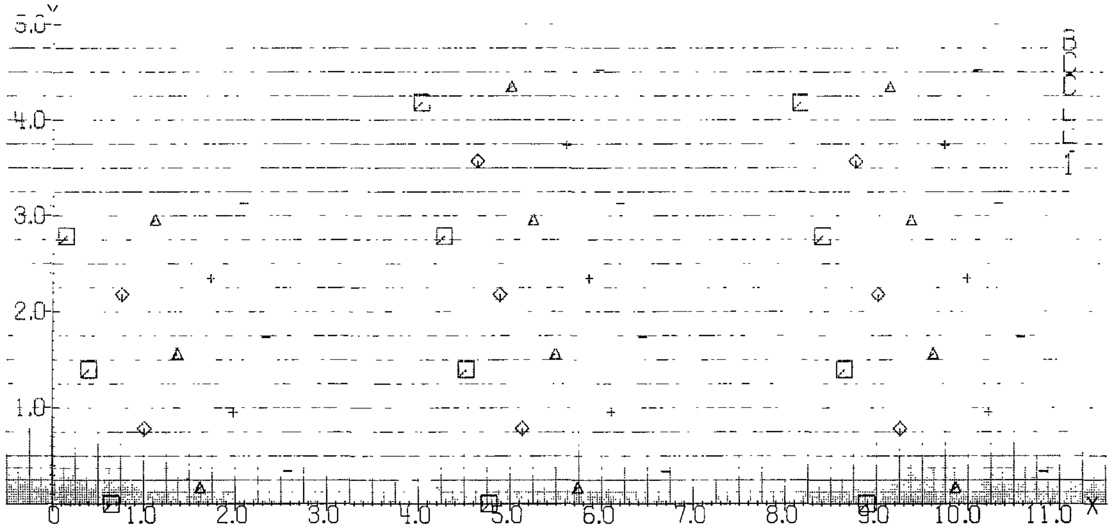


Figure 57. - Body-centered-cubic structure; 443 plane.



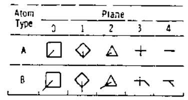


Figure 58. - Body-centered-cubic structure; 441 plane.

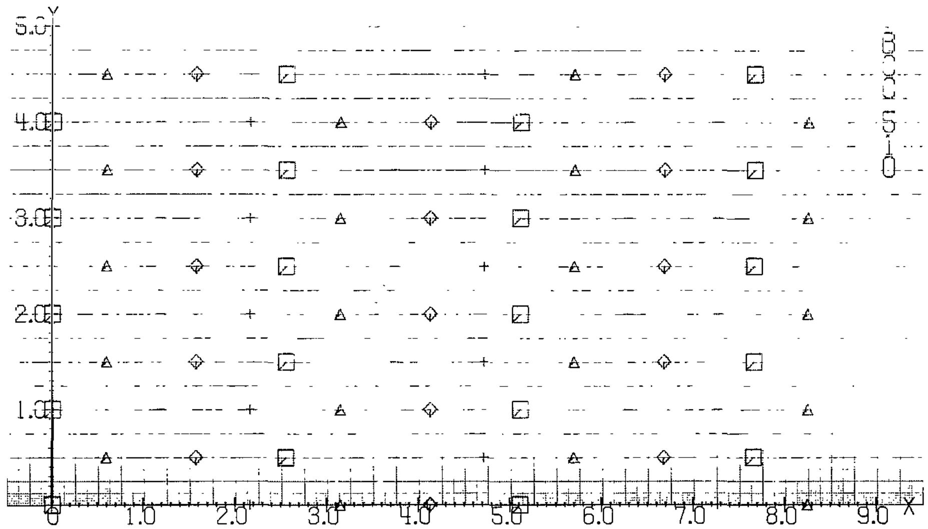


Figure 59. - Body-centered-cubic structure; 510 plane.

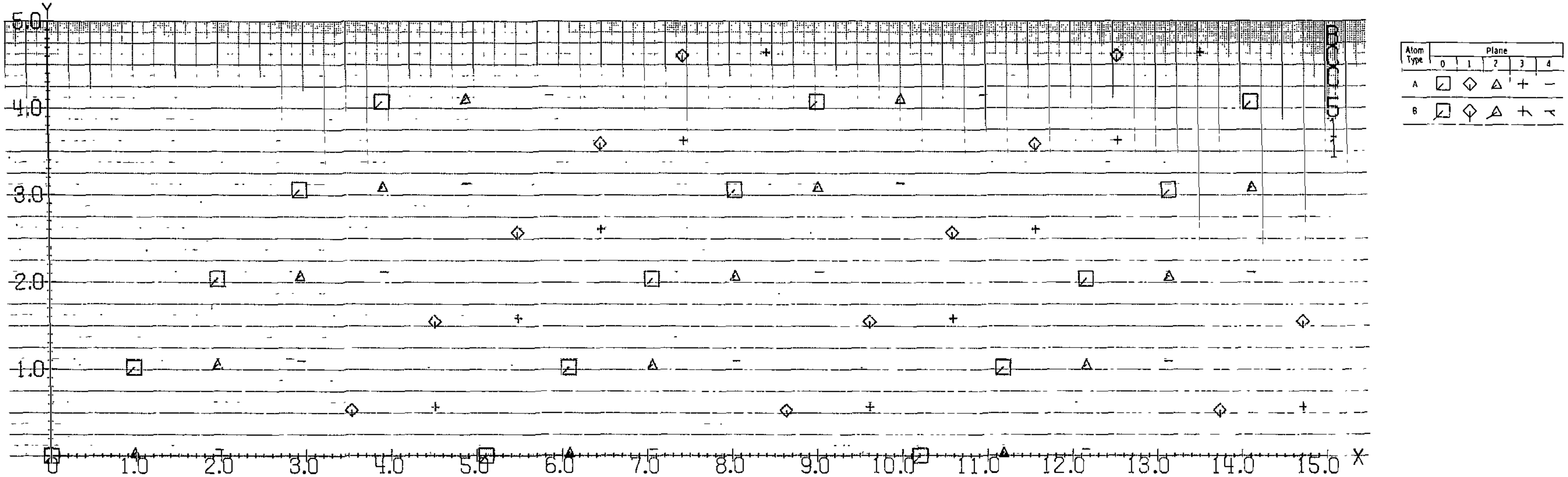


Figure 60. - Body-centered-cubic structure; 511 plane.

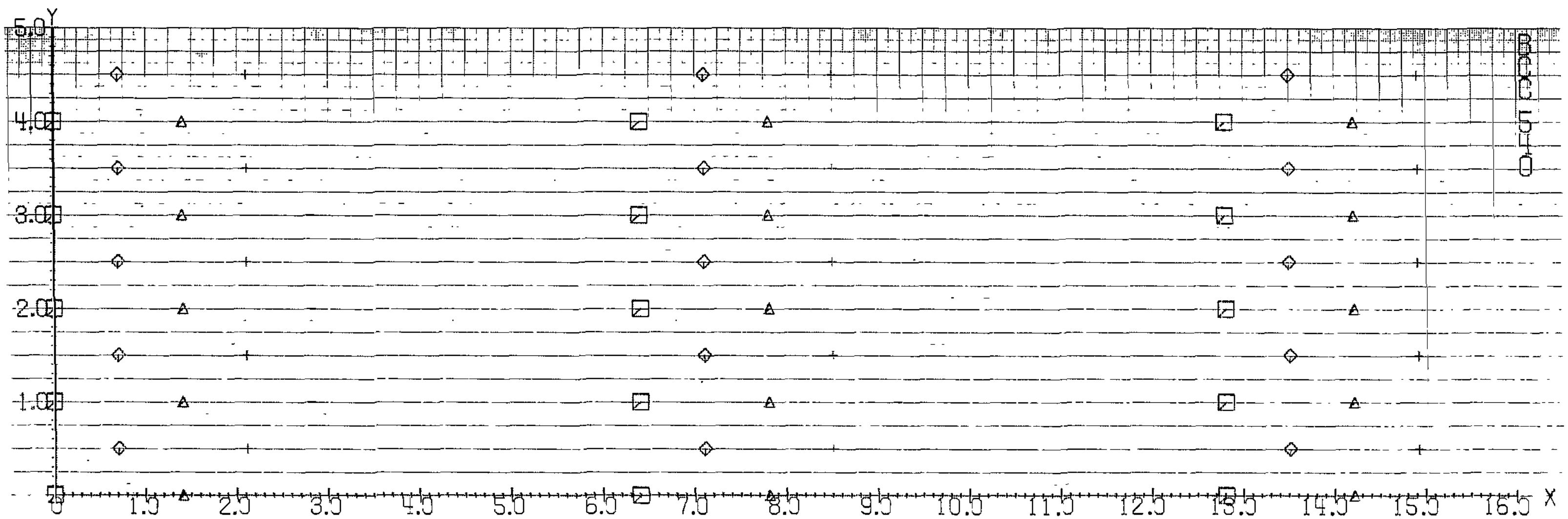


Figure 61. - Body-centered-cubic structure; 540 plane.

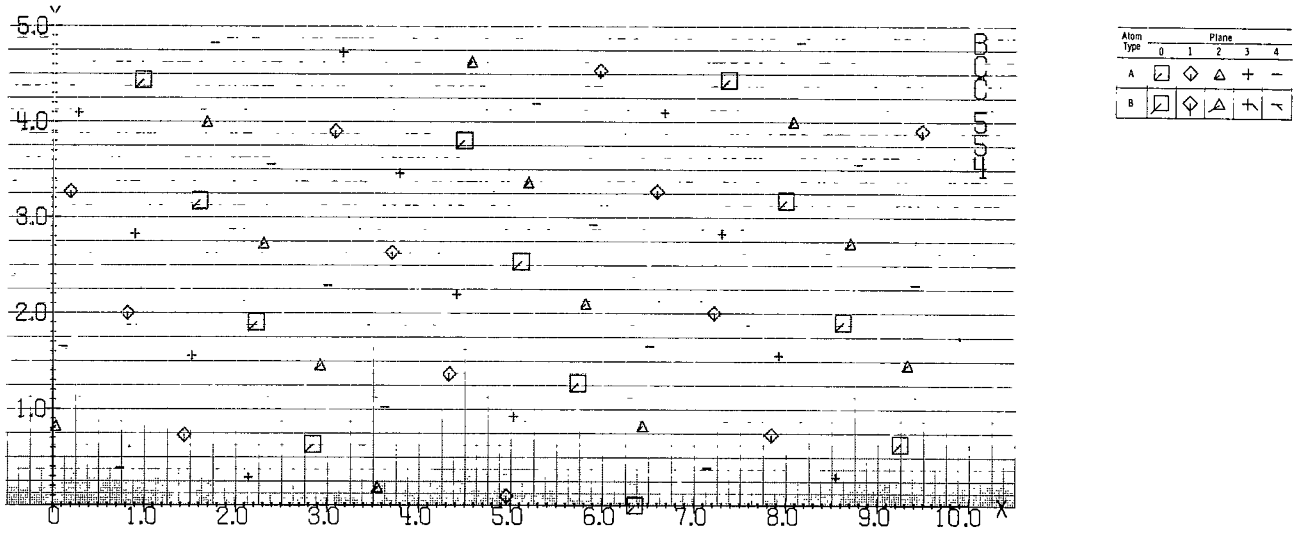


Figure 62. - Body-centered-cubic structure; 554 plane.

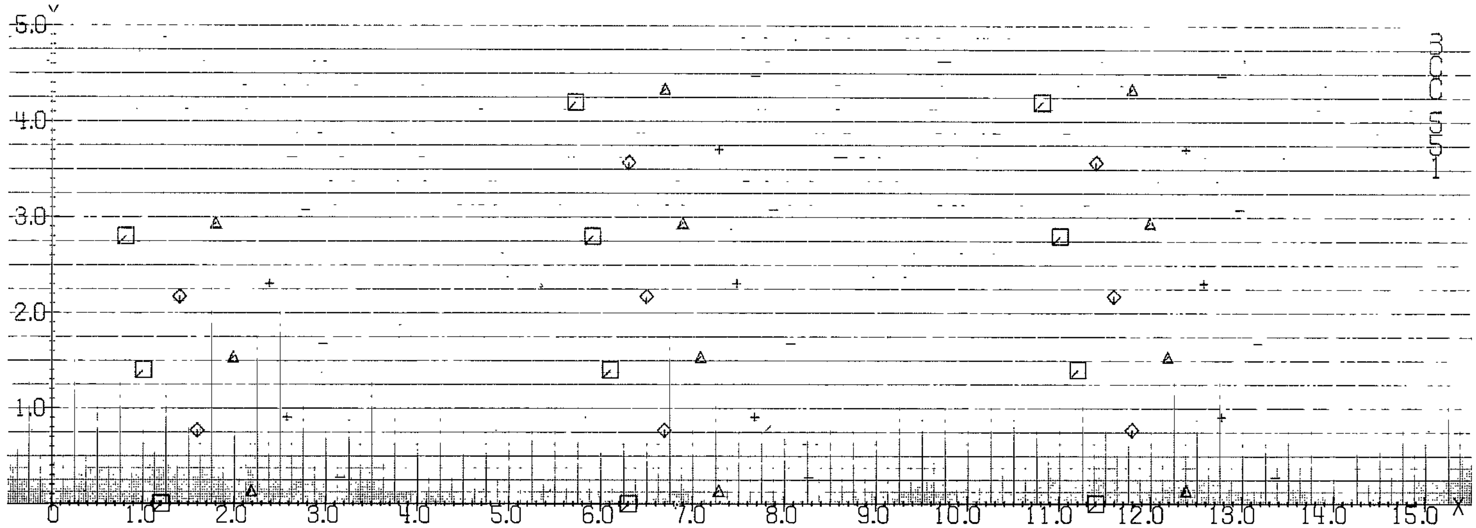


Figure 63. - Body-centered-cubic structure; 551 plane.

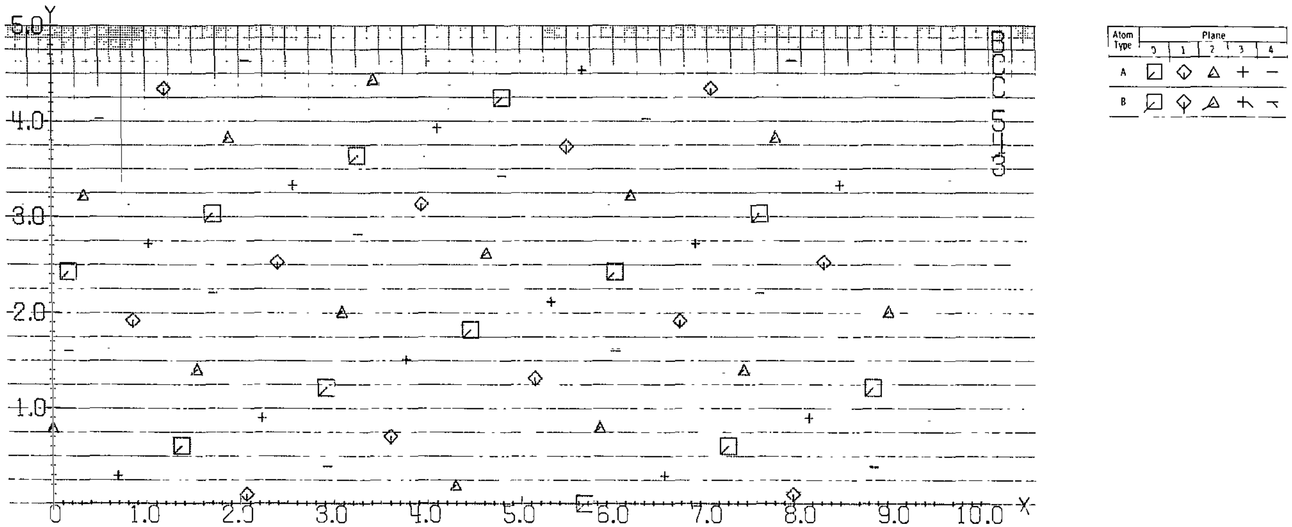


Figure 64. - Body-centered-cubic structure; 543 plane.

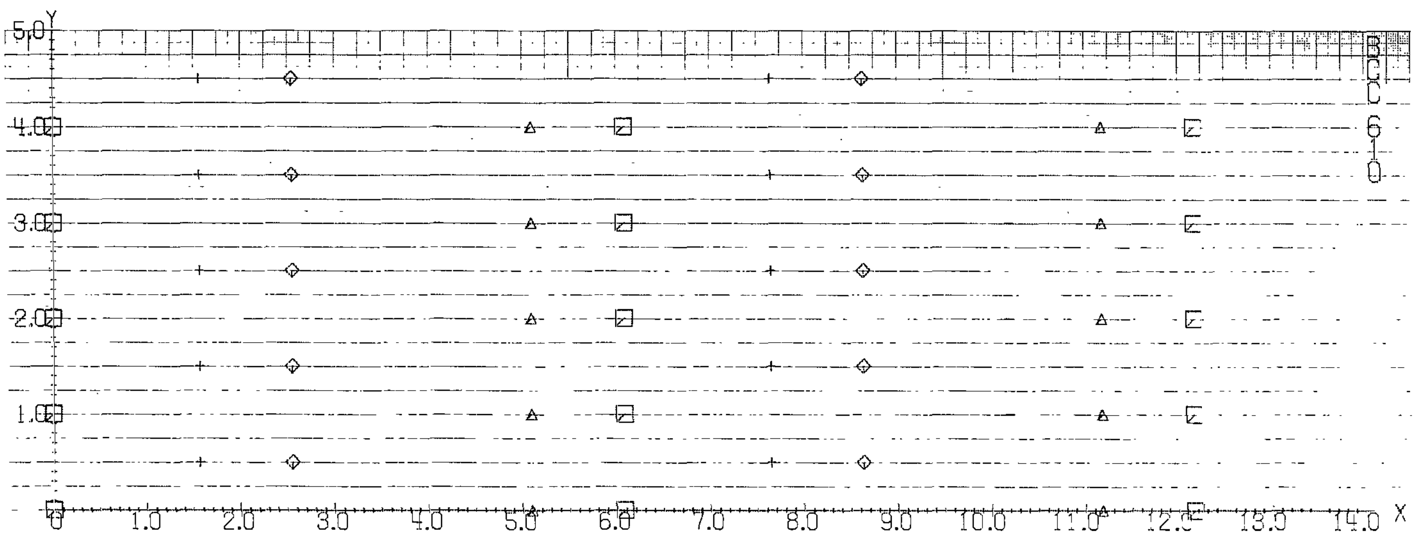


Figure 65. - Body-centered-cubic structure; 610 plane.

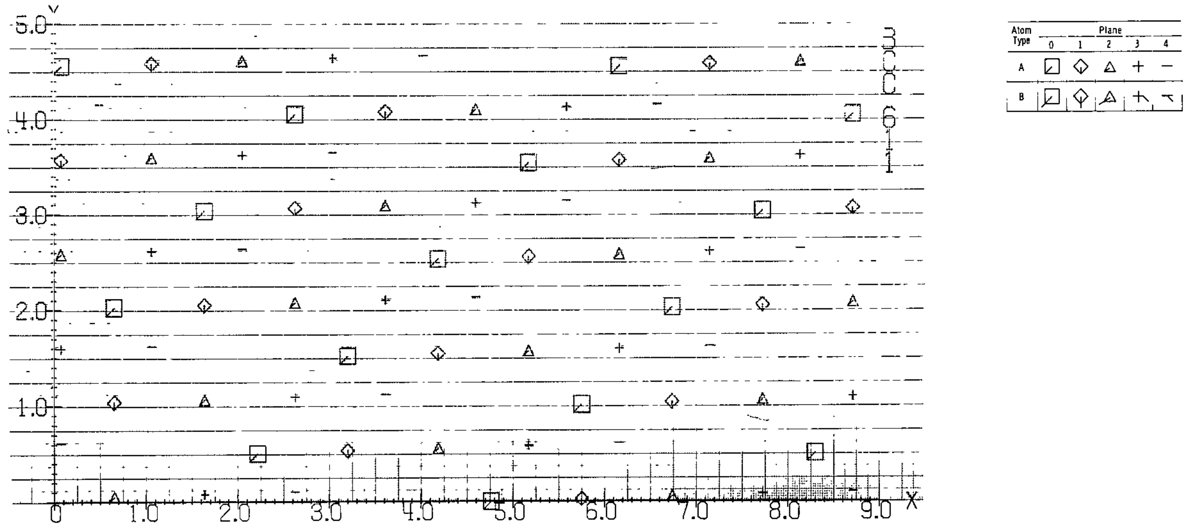


Figure 66. - Body-centered-cubic structure; 611 plane.

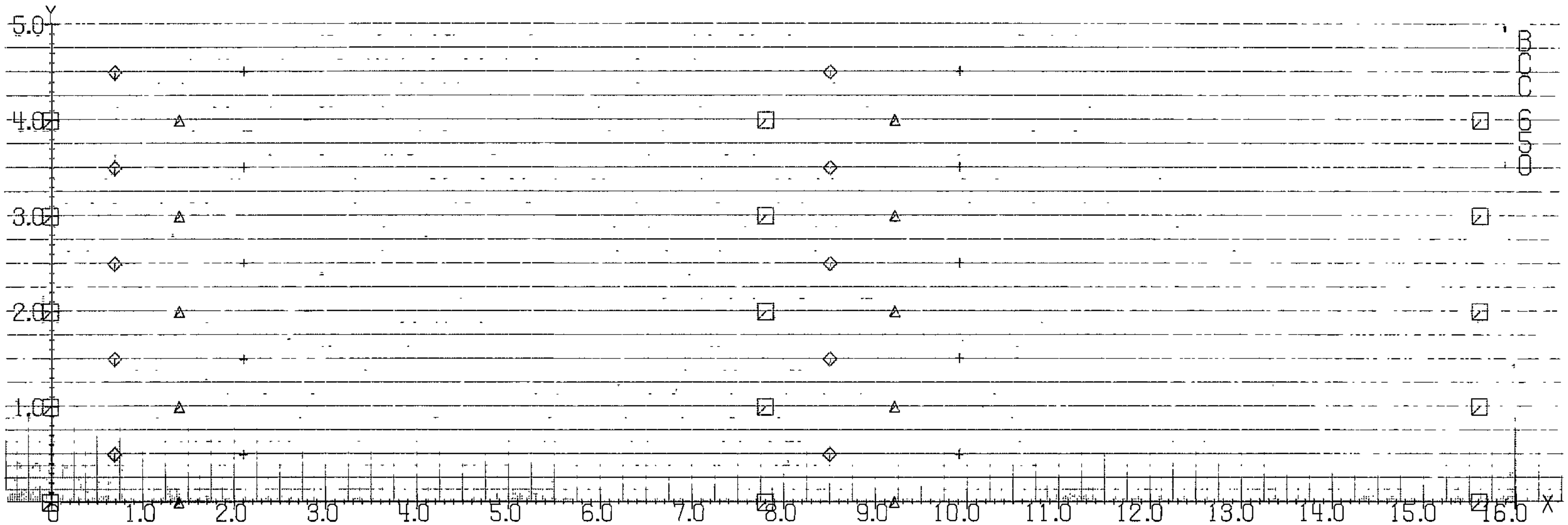


Figure 67. - Body-centered-cubic structure; 650 plane.

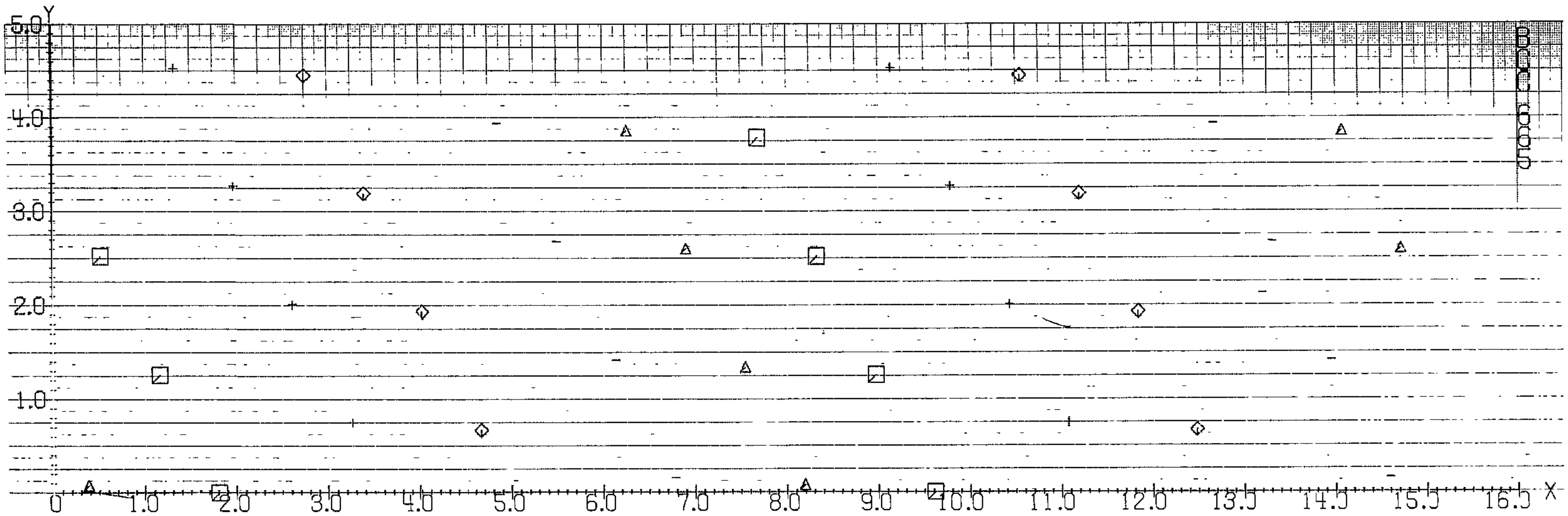
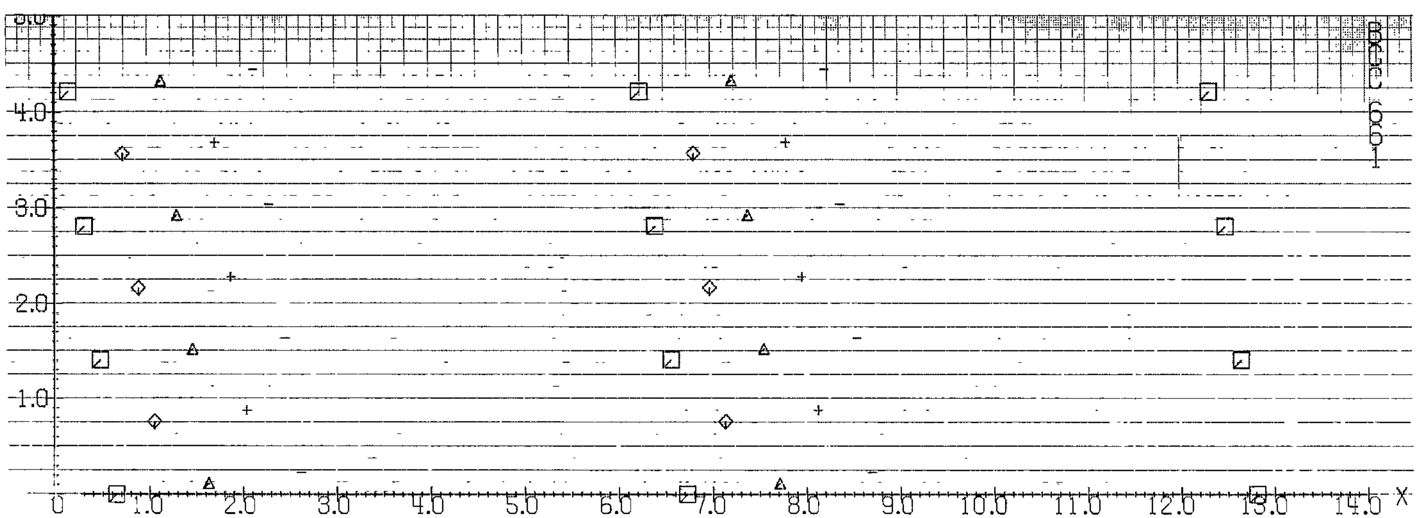


Figure 68. - Body-centered-cubic structure; 665 plane.



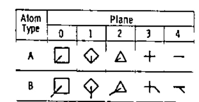


Figure 69. - Body-centered-cubic structure; 661 plane.

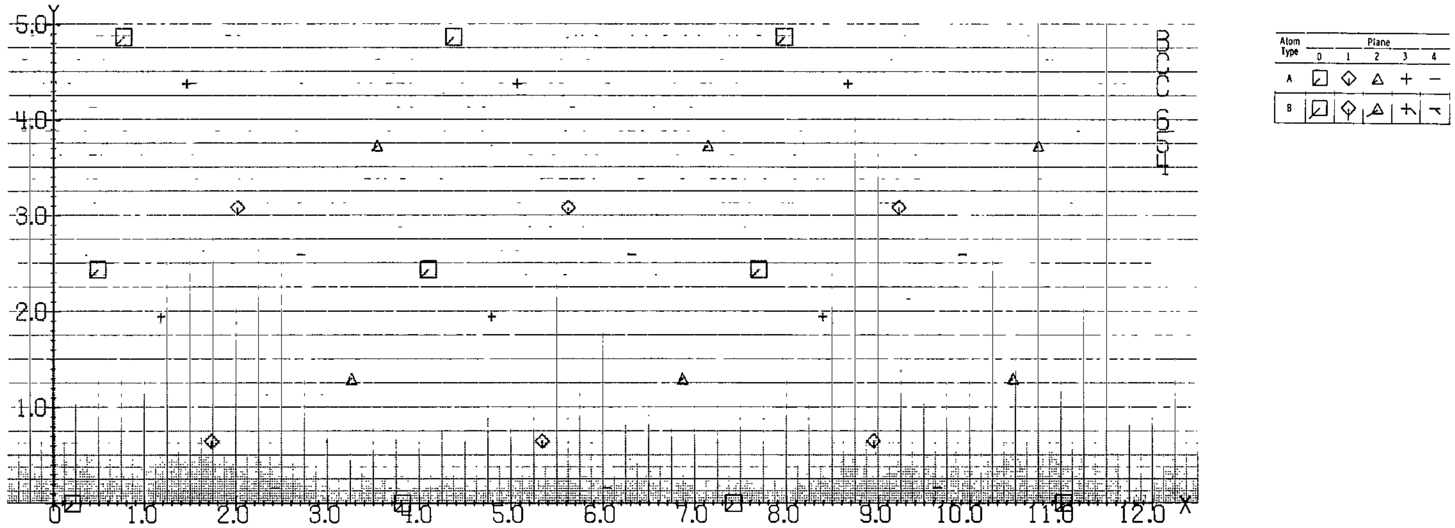


Figure 70. - Body-centered-cubic structure; 654 plane.

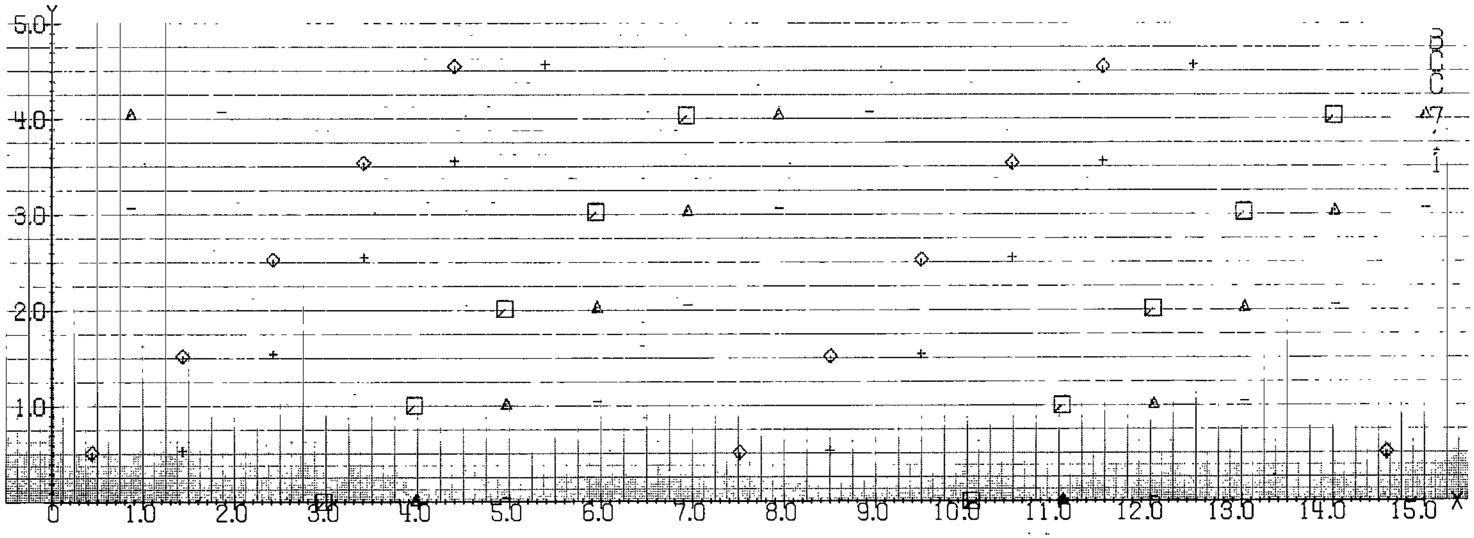


Figure 71. - Body-centered-cubic structure; 711 plane.

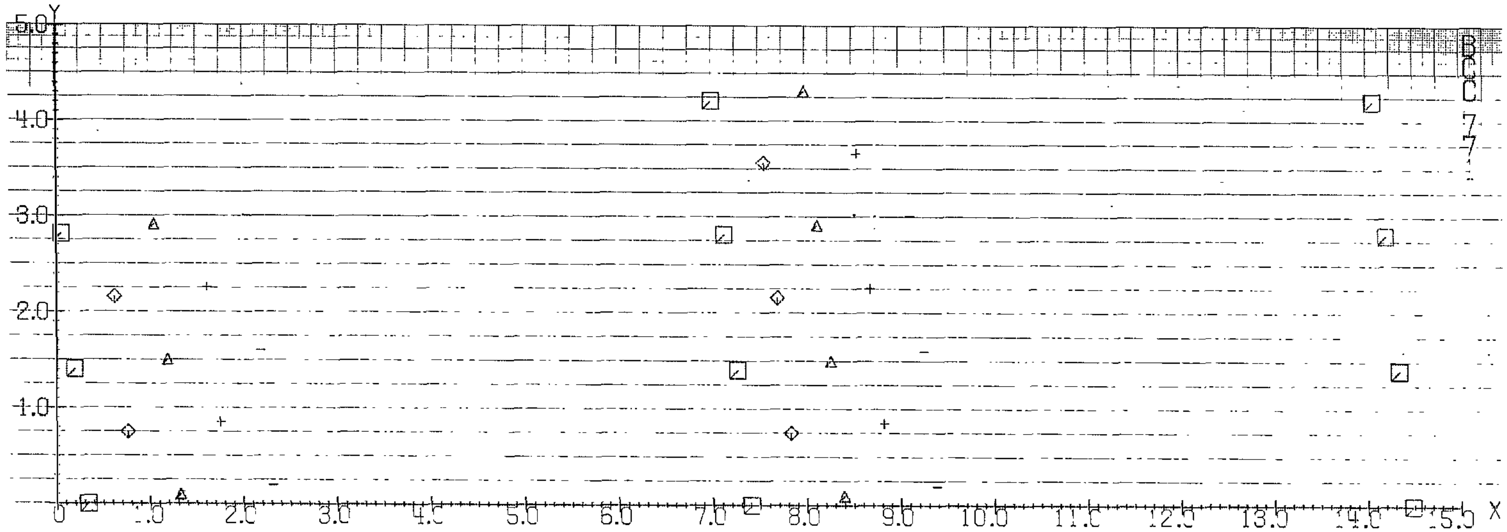
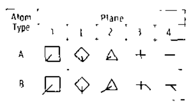


Figure 72. - Body-centered-cubic structure; 771 plane.



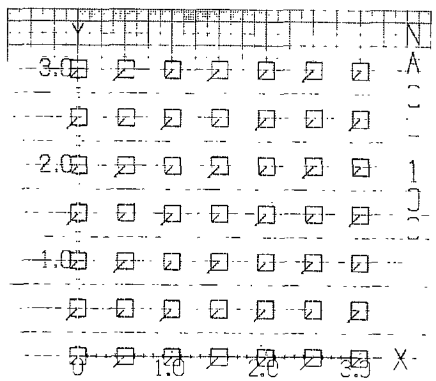


Figure 73. - Sodium chloride structure; 100 plane.

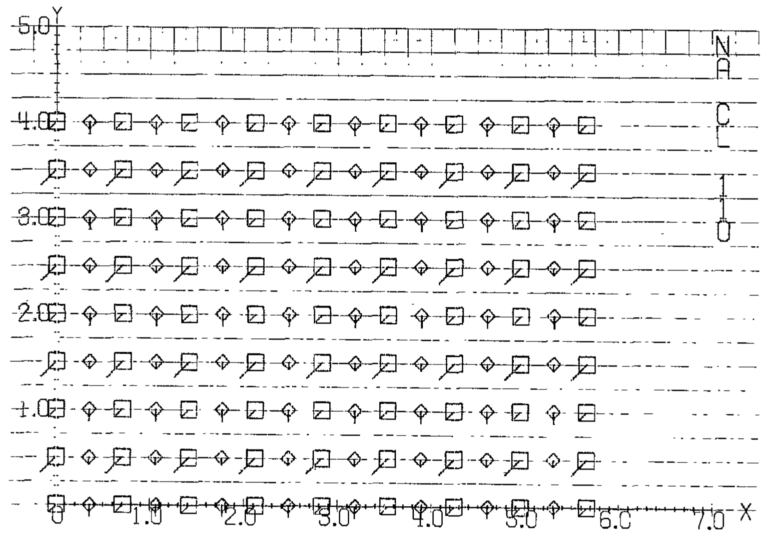


Figure 74. - Sodium chloride structure; 110 plane.

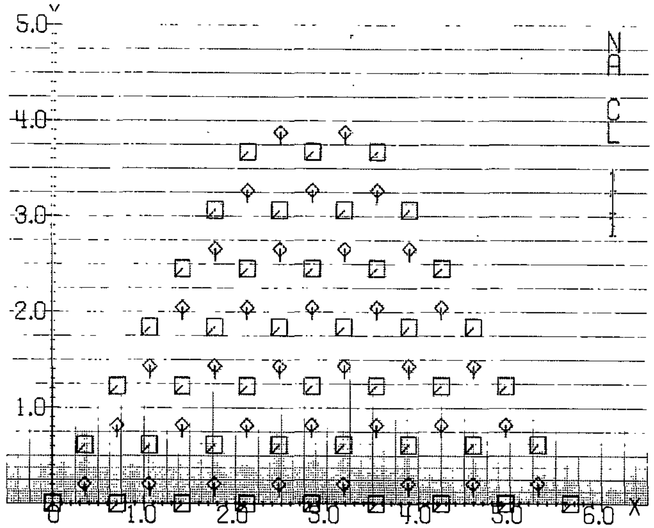


Figure 75. - Sodium chloride structure; 111 plane.

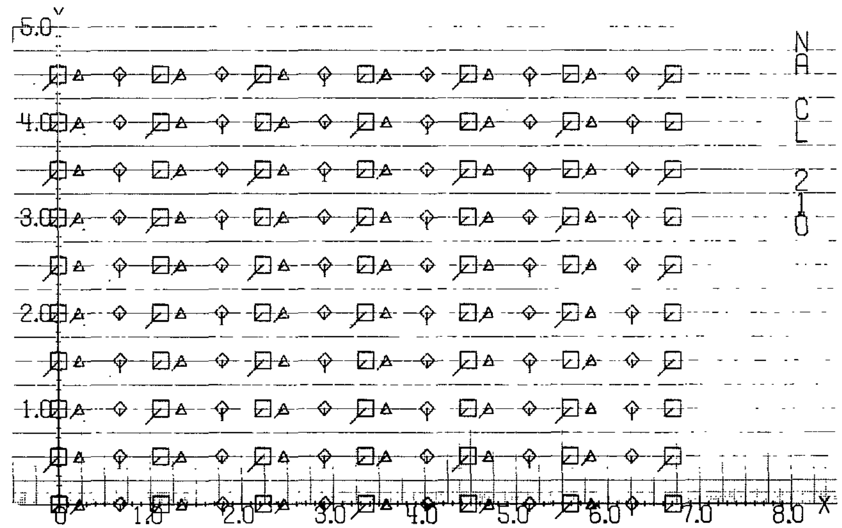


Figure 76. - Sodium chloride structure; 210 plane.

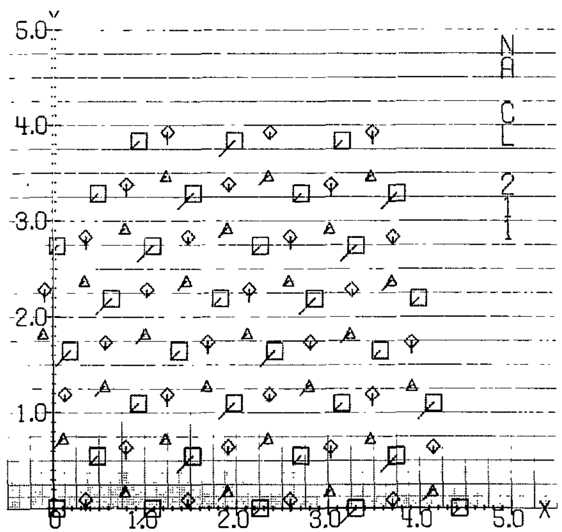


Figure 77. - Sodium chloride structure; 211 plane.

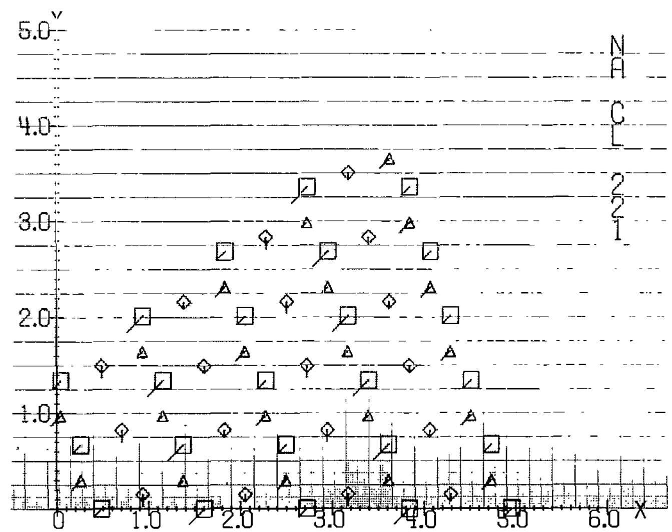
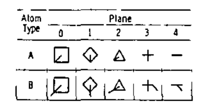
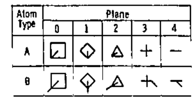


Figure 78. - Sodium chloride structure; 221 plane.





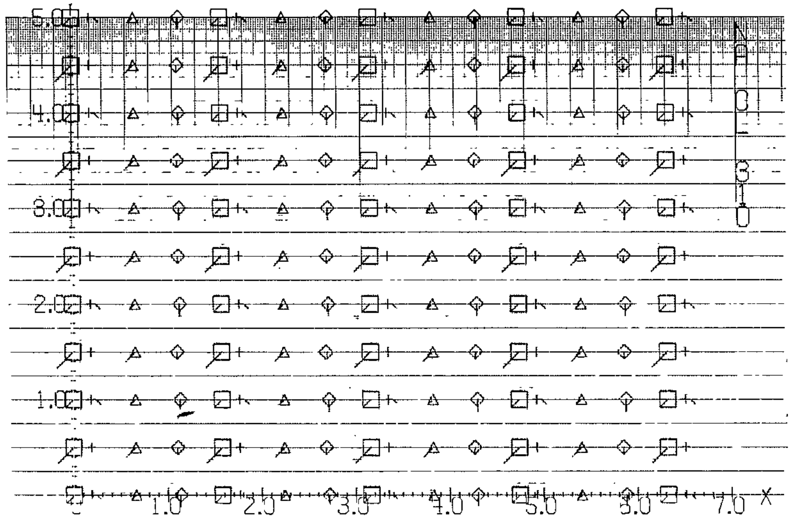


Figure 79. - Sodium chloride structure; 310 plane.

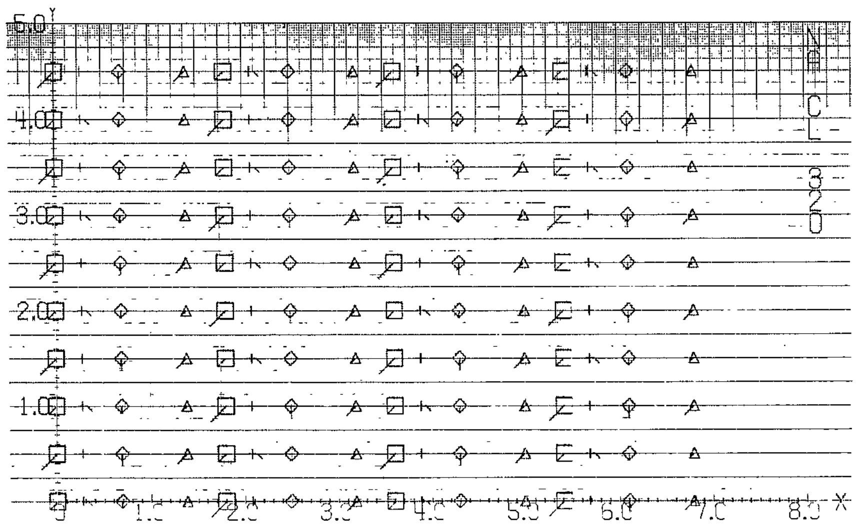


Figure 80. - Sodium chloride structure; 320 plane.

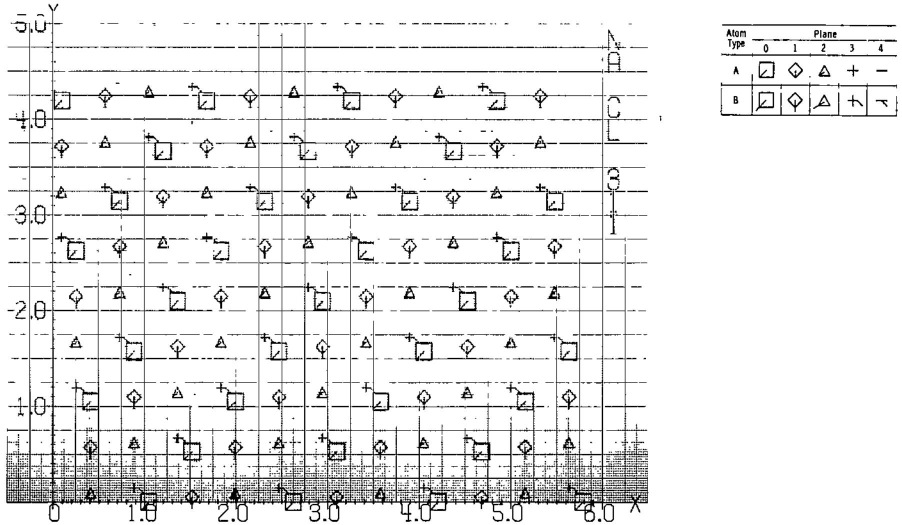


Figure 81. - Sodium chloride structure; 311 plane.

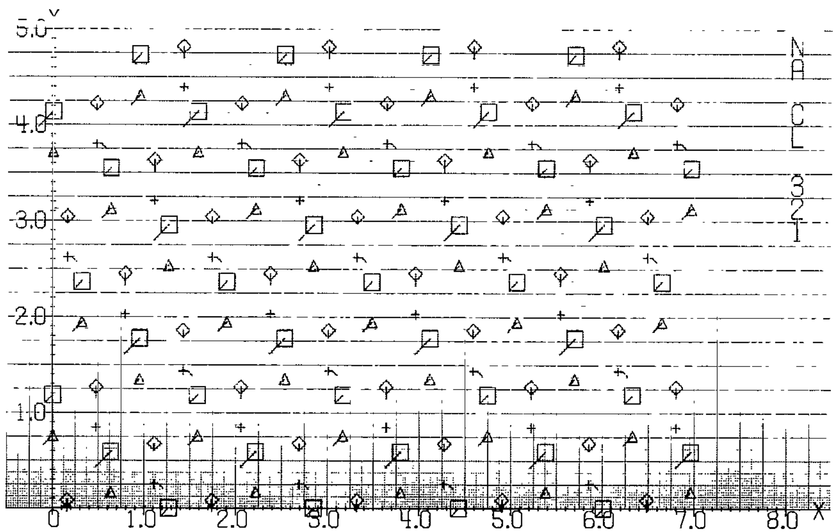
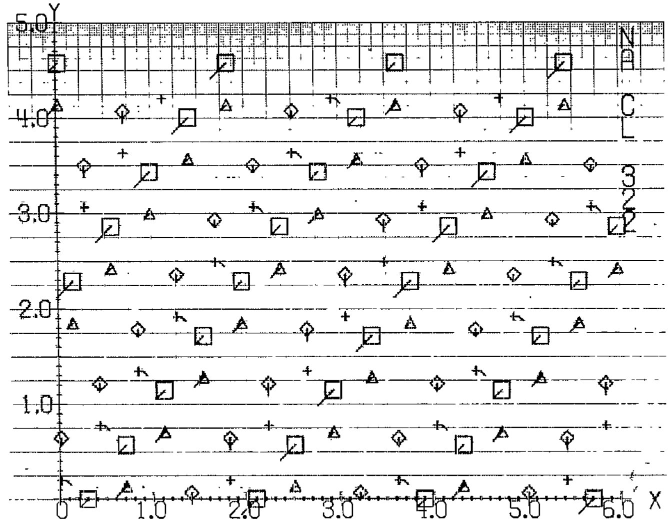


Figure 82. - Sodium chloride structure; 321 plane.



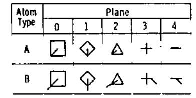


Figure 83. - Sodium chloride structure; 322 plane.

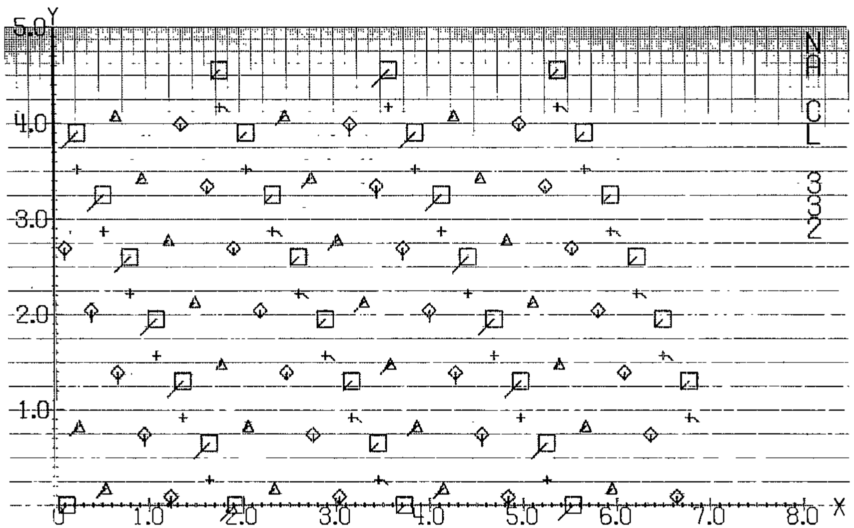


Figure 84. - Sodium chloride structure; 332 plane.

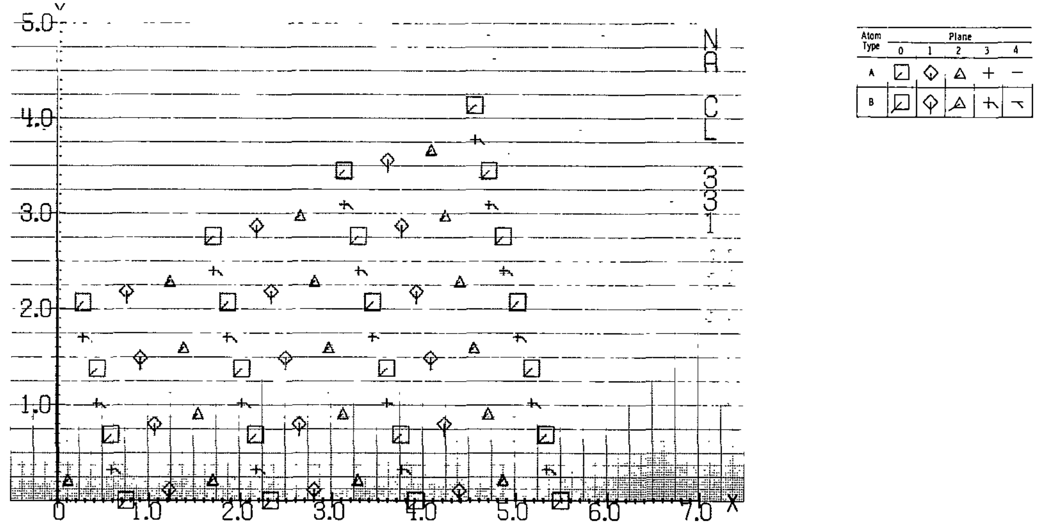


Figure 85. - Sodium chloride structure; 331 plane.

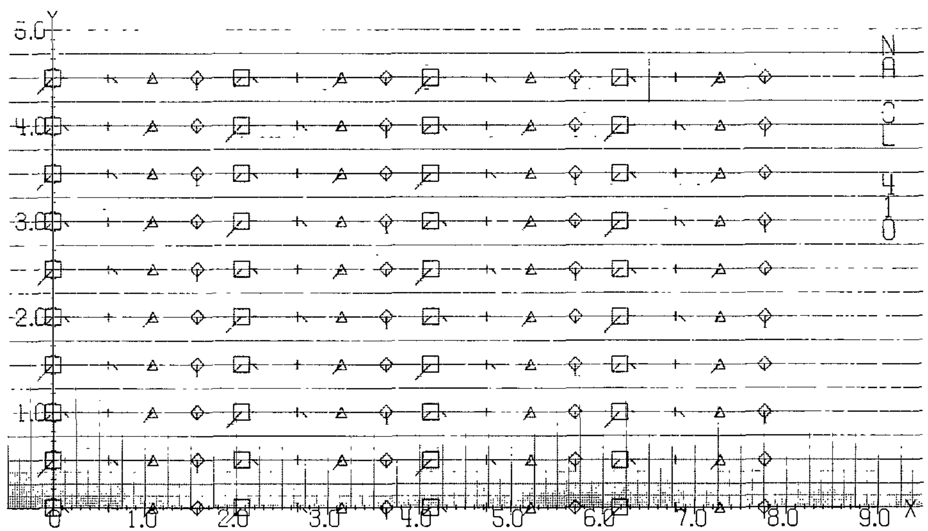
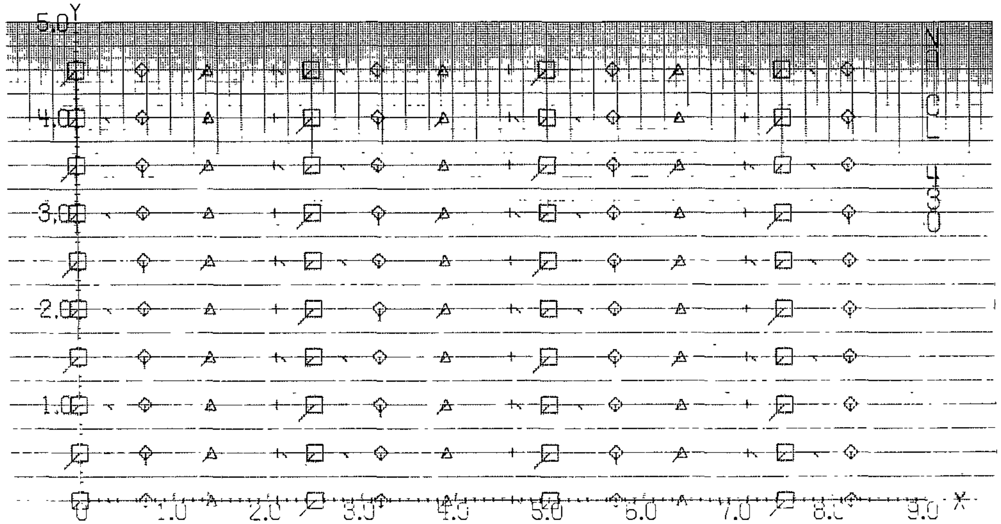


Figure 86. - Sodium chloride structure; 410 plane.



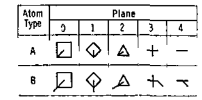


Figure 87. - Sodium chloride structure; 430 plane.

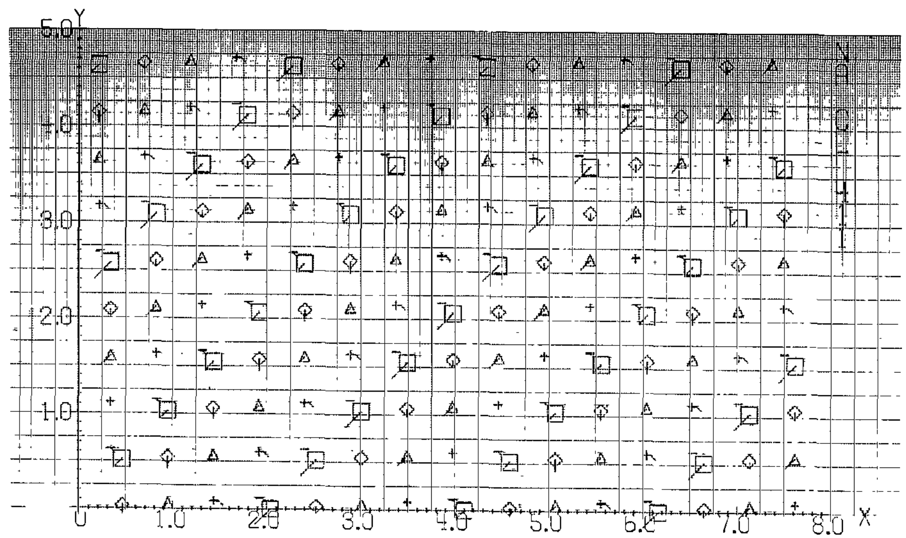


Figure 88. - Sodium chloride structure; 411 plane.

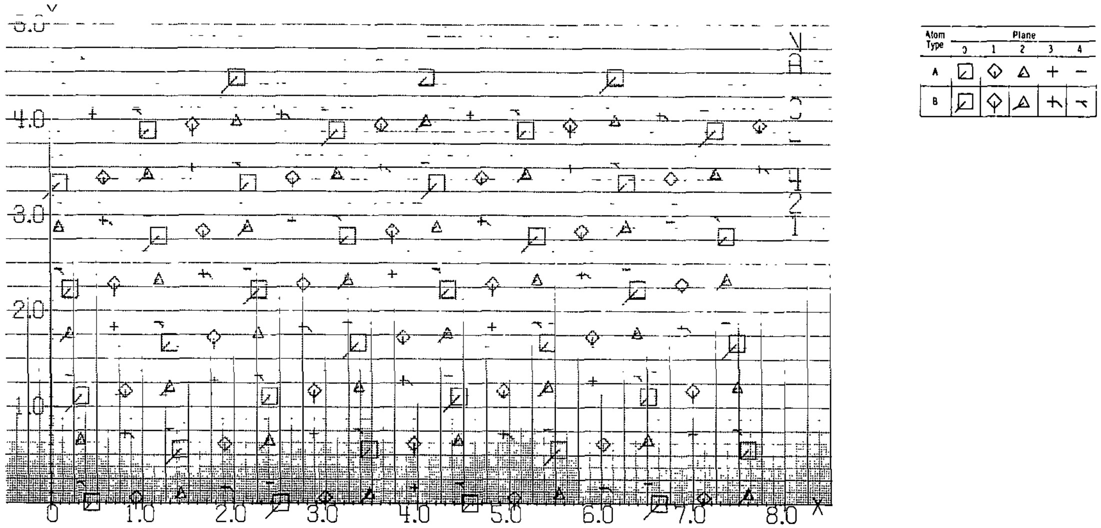


Figure 89. - Sodium chloride structure; 421 plane.

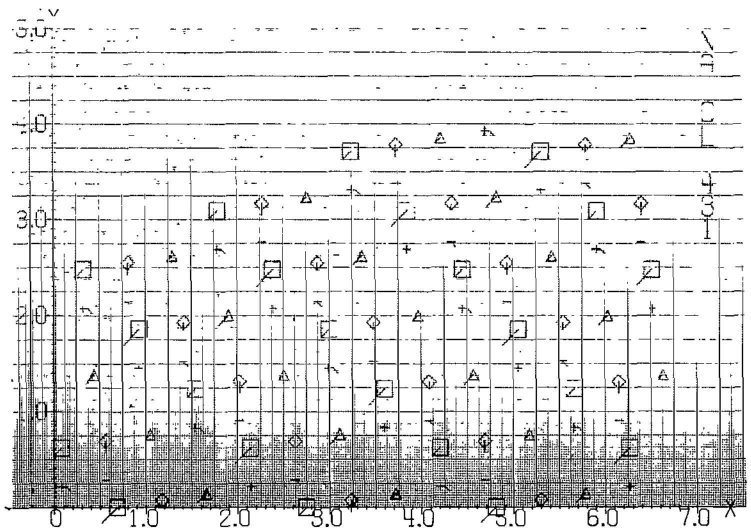
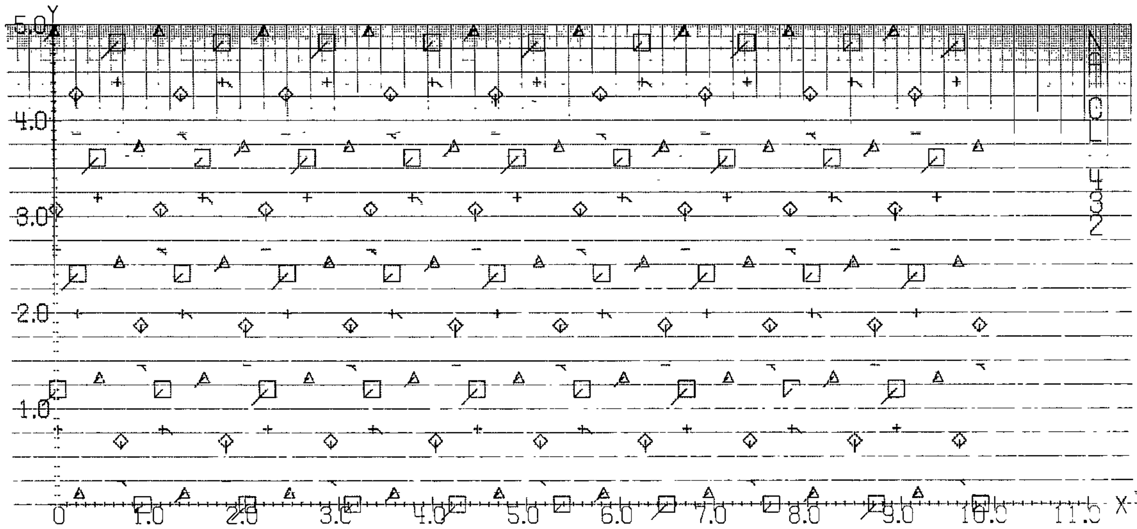


Figure 90. - Sodium chloride structure; 431 plane.



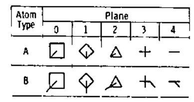


Figure 91. - Sodium chloride structure; 432 plane.

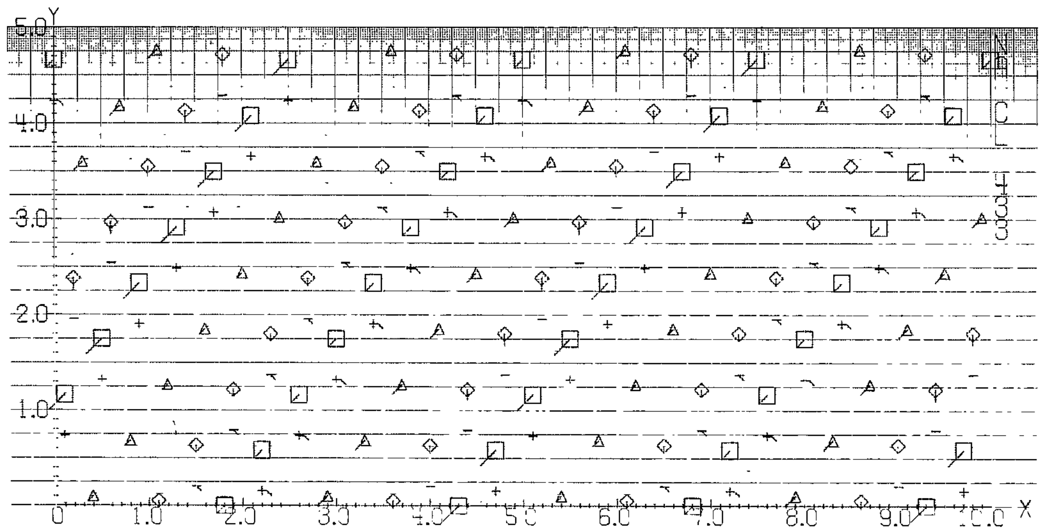


Figure 92. - Sodium chloride structure; 433 plane.

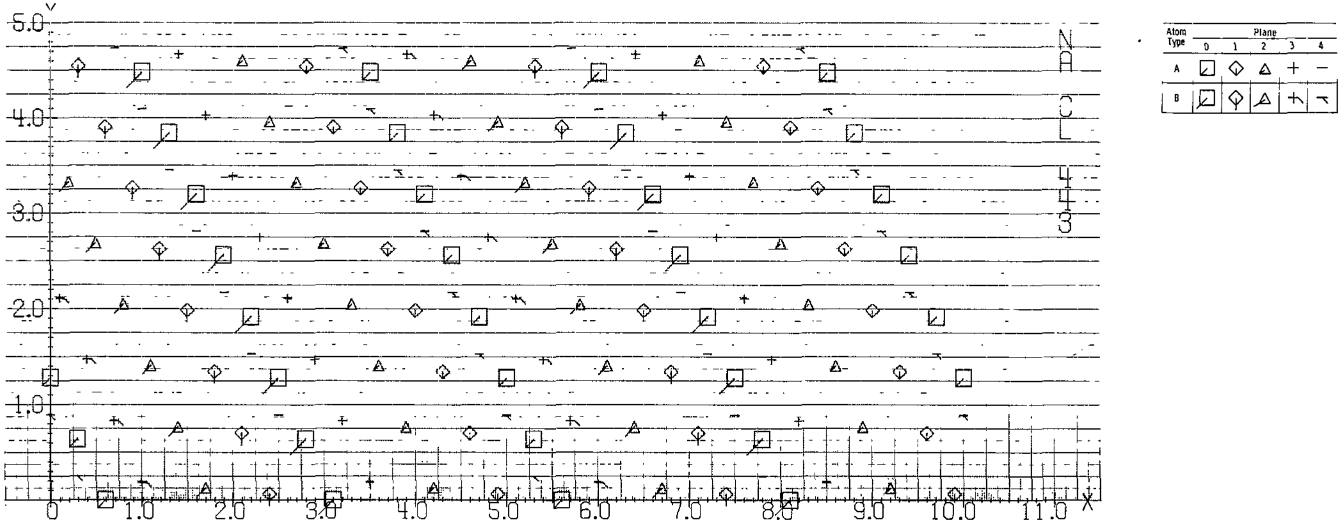


Figure 93. - Sodium chloride structure; 443 plane.

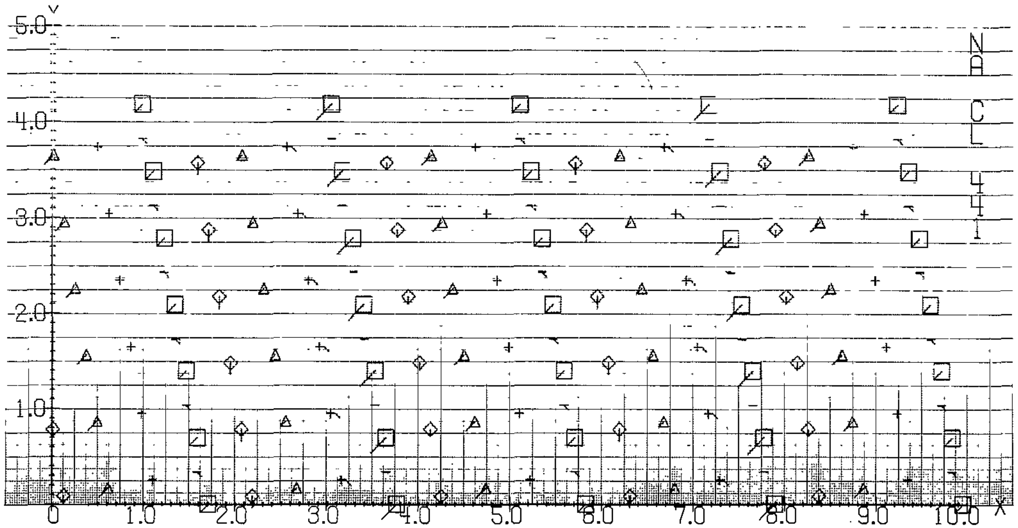


Figure 94. - Sodium chloride structure; 441 plane.

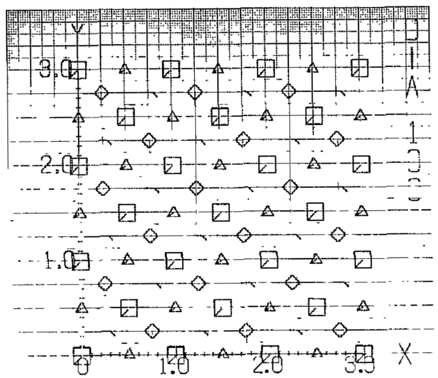


Figure 95. - Diamond structure; 100 plane.

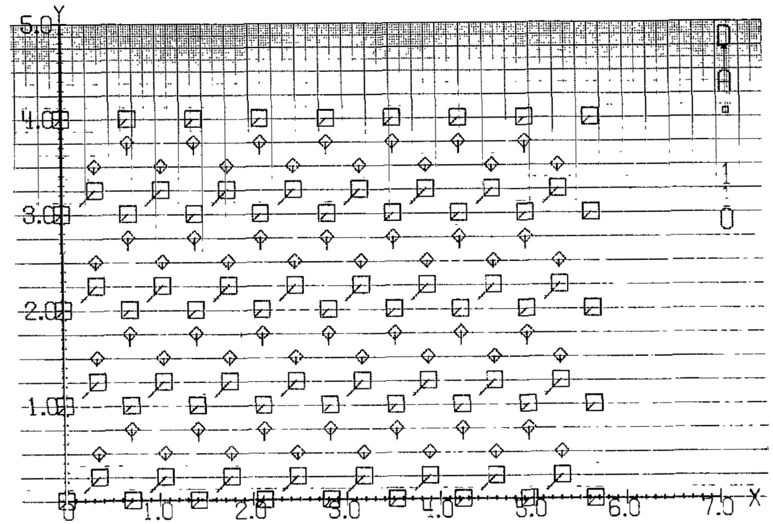


Figure 96. - Diamond structure; 110 plane.

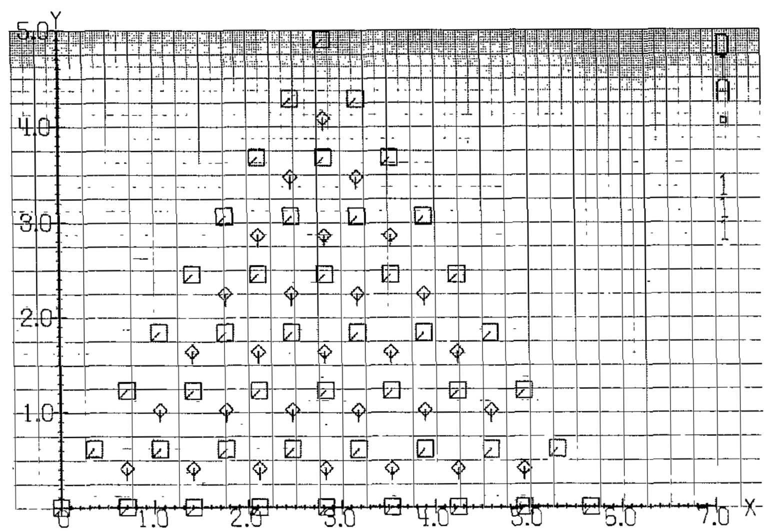
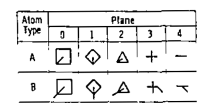


Figure 97. - Diamond structure; 111 plane.



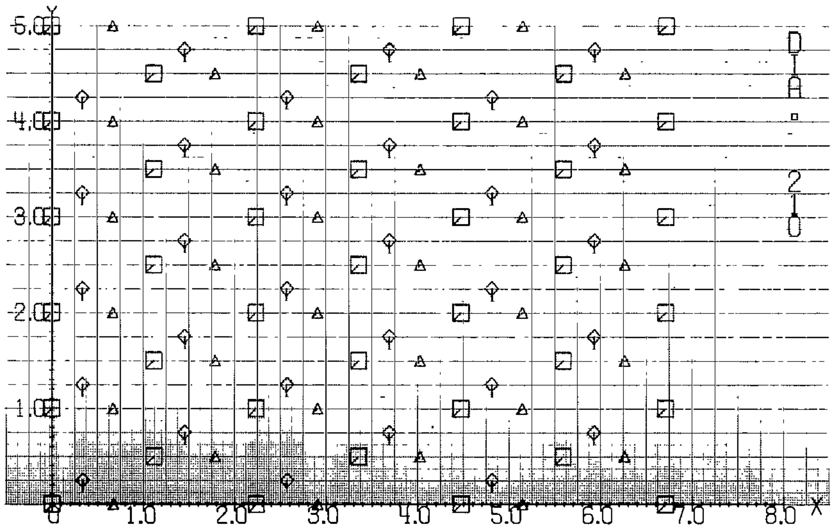


Figure 98. - Diamond structure; 210 plane.

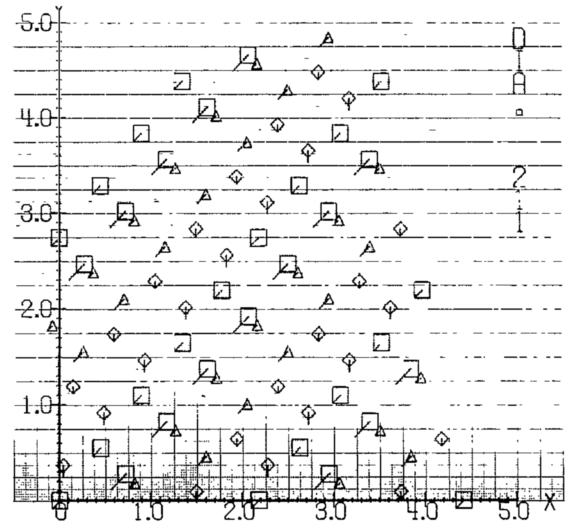


Figure 99. - Diamond structure; 211 plane.

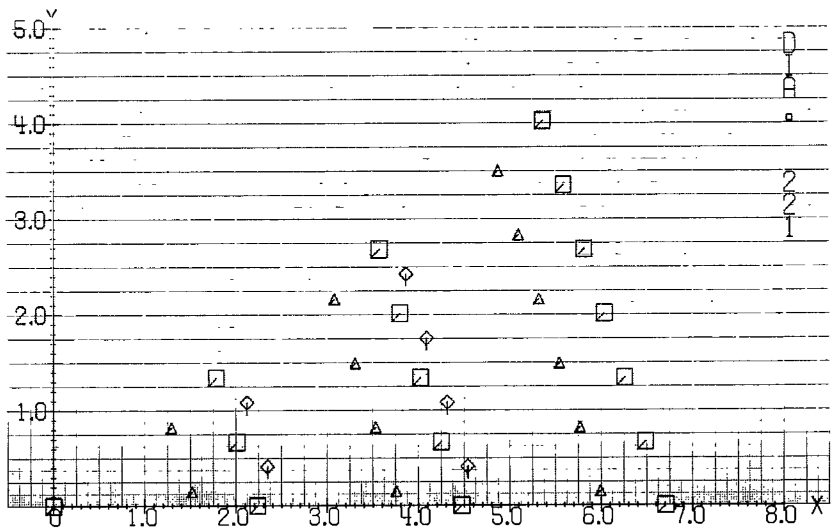
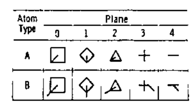


Figure 100. - Diamond structure; 221 plane.



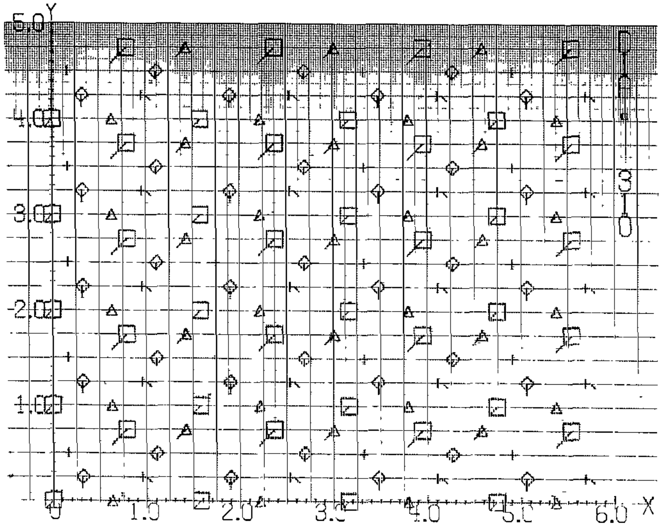


Figure 101. - Diamond structure; 310 plane.

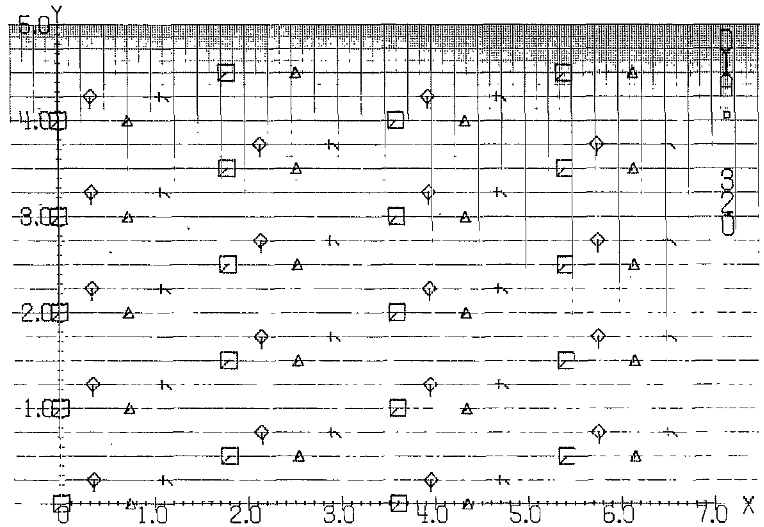


Figure 102. - Diamond structure; 320 plane.

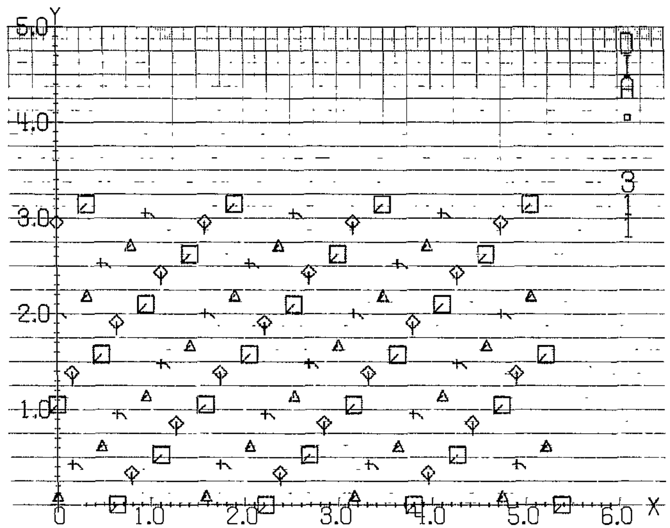
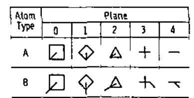


Figure 103. - Diamond structure; 311 plane.



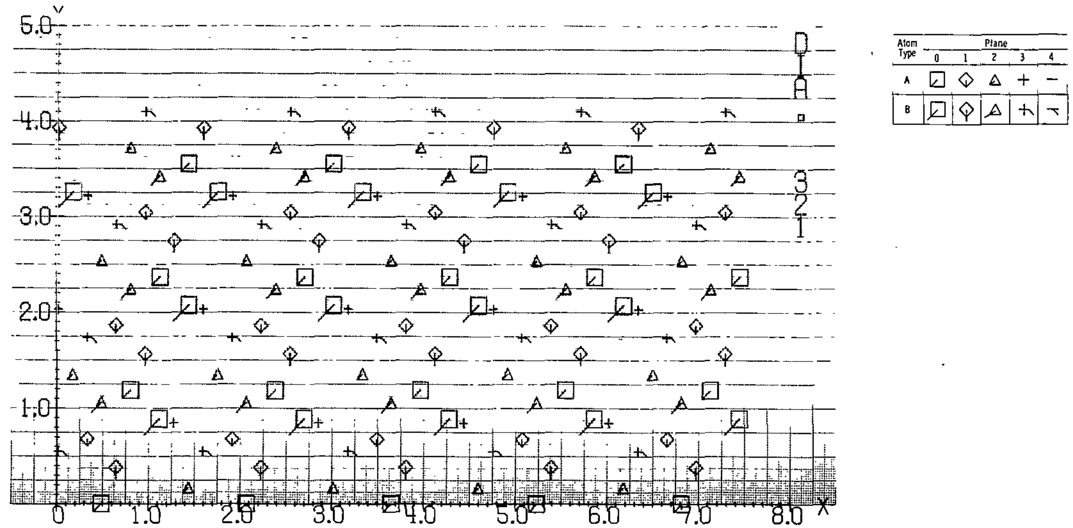


Figure 104. - Diamond structure; 321 plane.

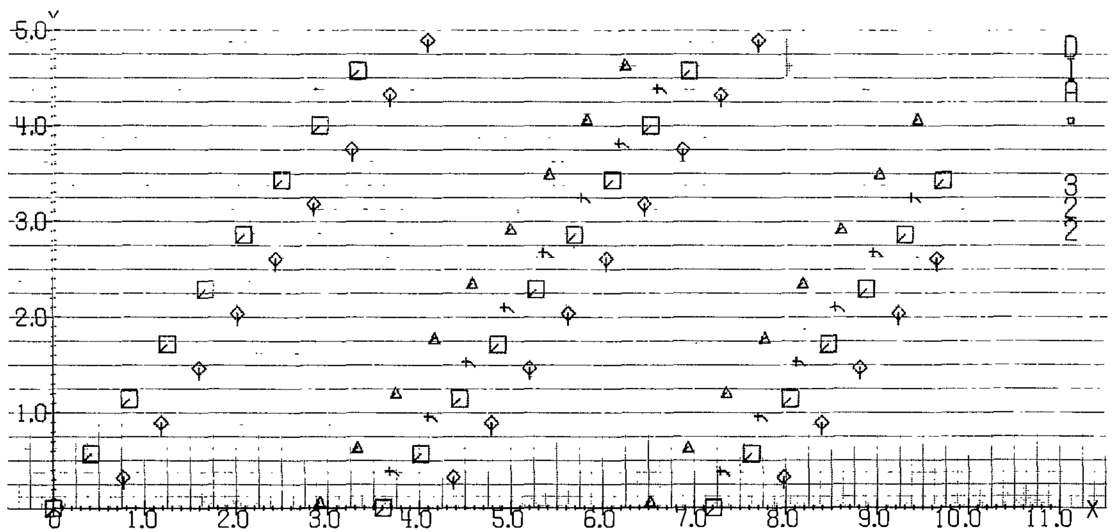


Figure 105. - Diamond structure; 322 plane.

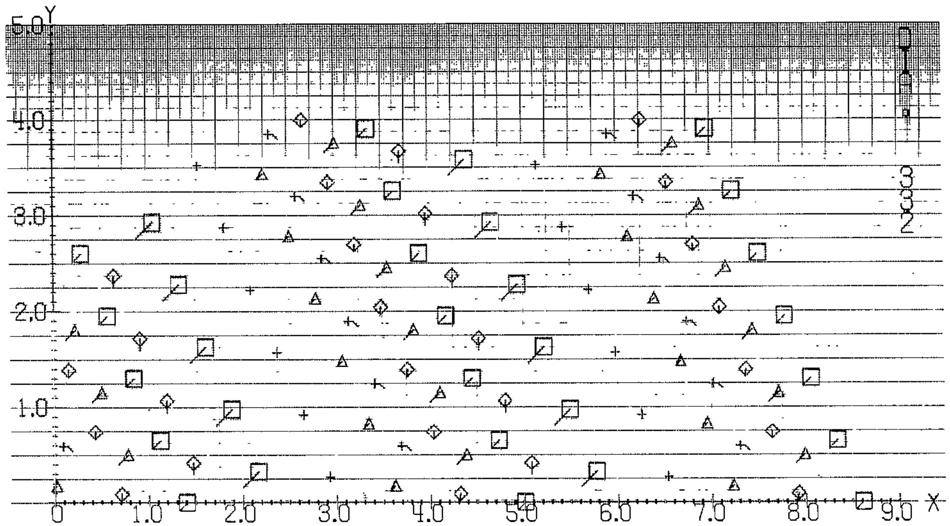
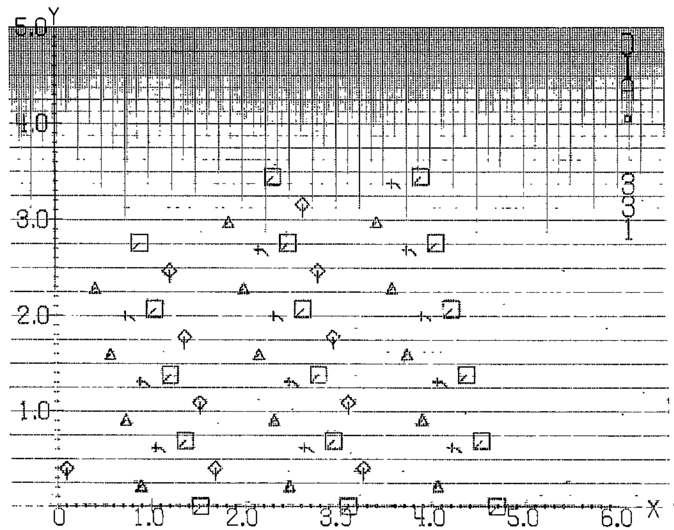


Figure 106. - Diamond structure; 332 plane.



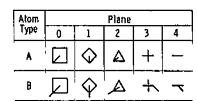
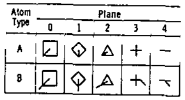


Figure 107. - Diamond structure; 331 plane.



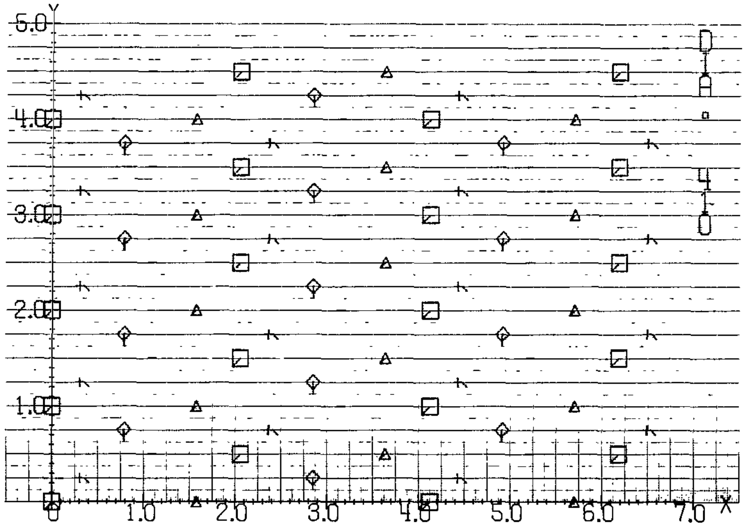


Figure 108. - Diamond structure; 410 plane.

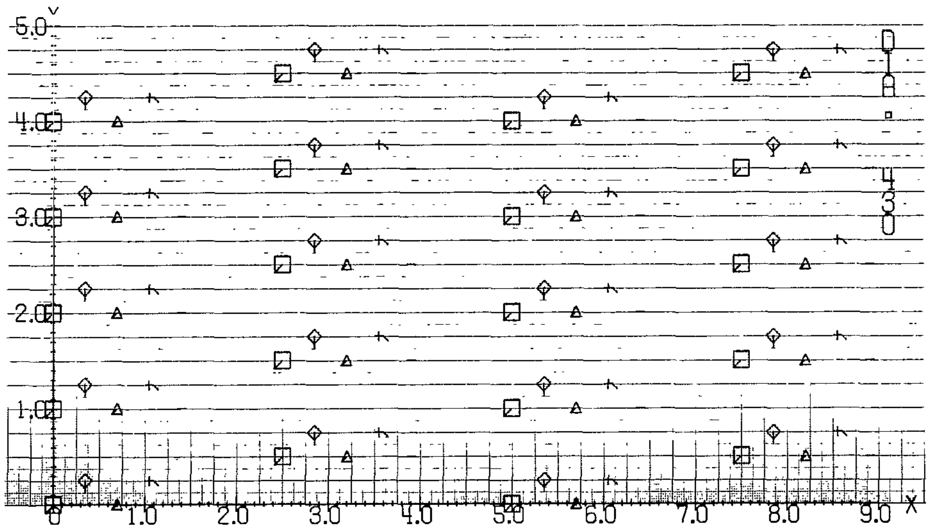


Figure 109. - Diamond structure; 430 plane.

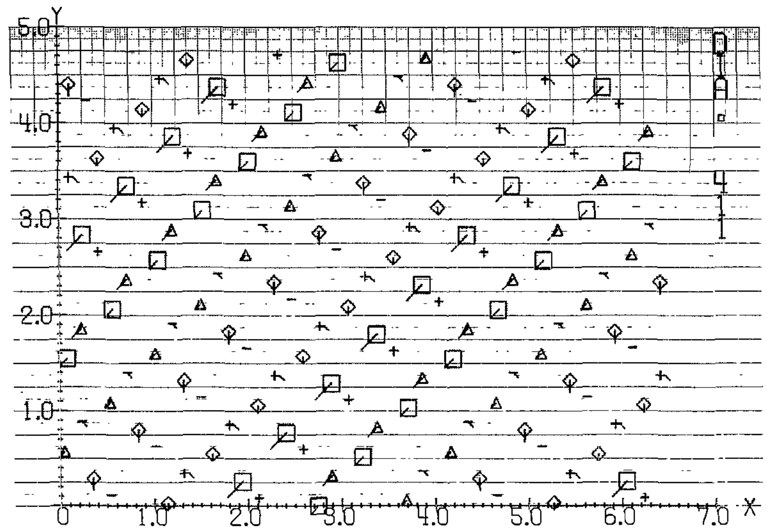
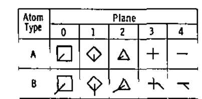


Figure 110. - Diamond structure; 411 plane.



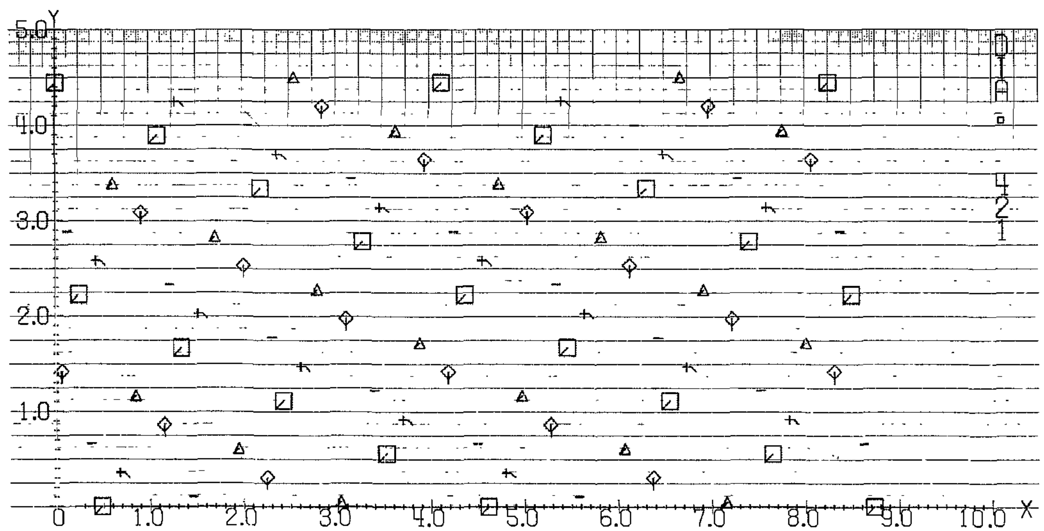


Figure 111. - Diamond structure; 421 plane.

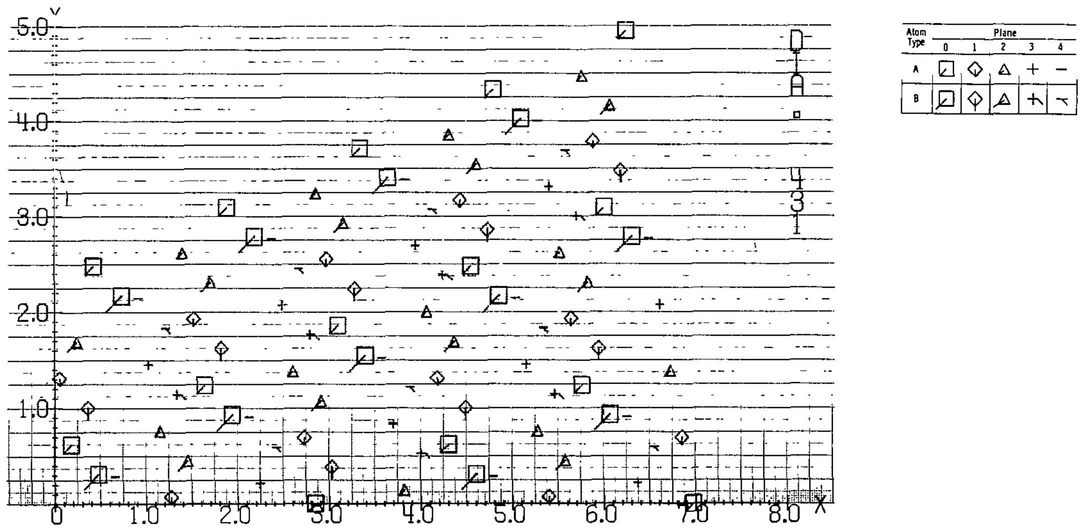


Figure 112. - Diamond structure; 431 plane.

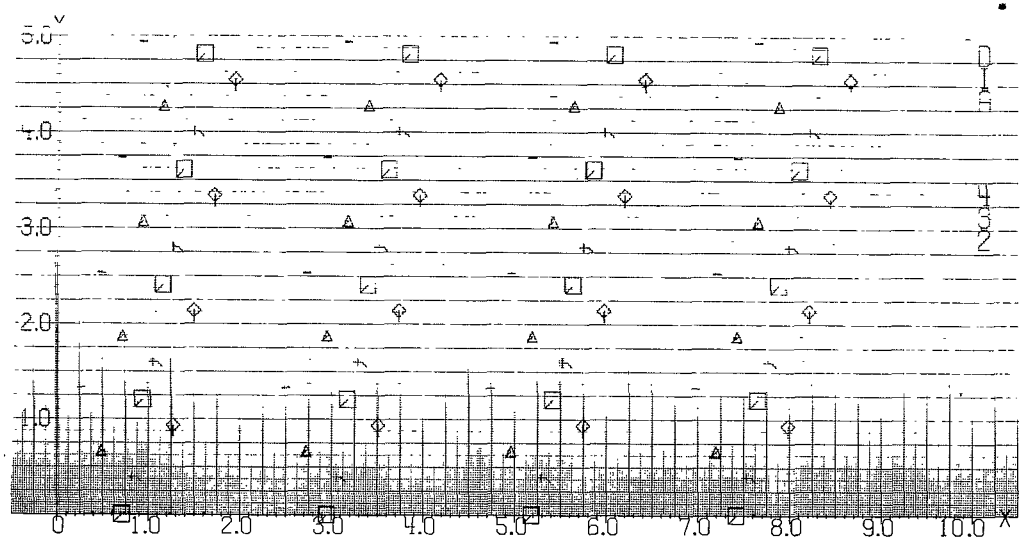


Figure 113. - Diamond structure; 432 plane.

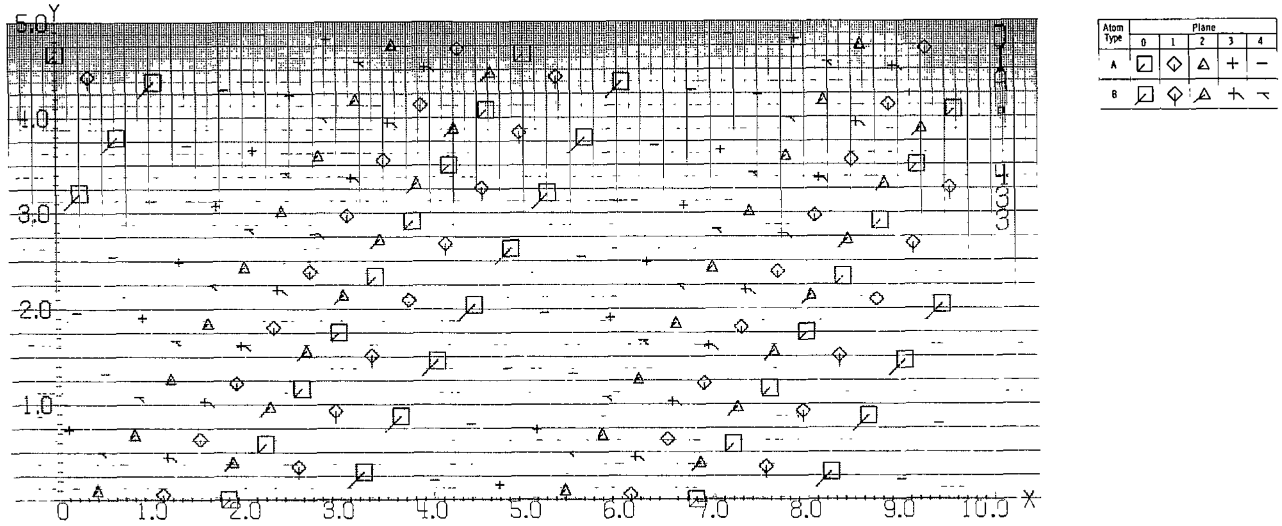


Figure 114. - Diamond structure; 433 plane.

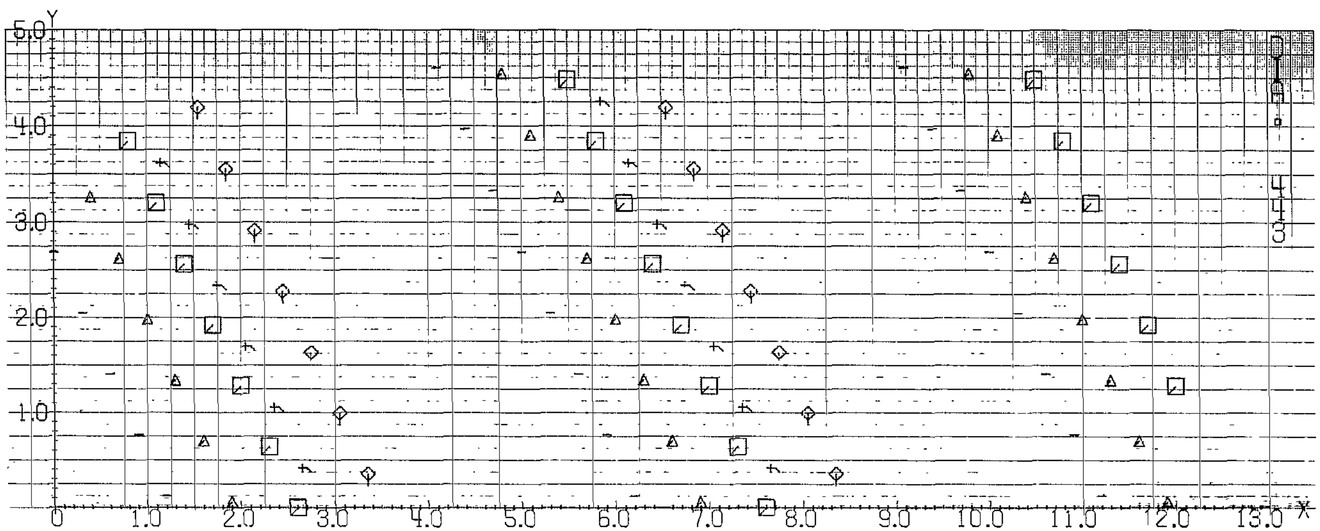


Figure 115. - Diamond structure; 443 plane.

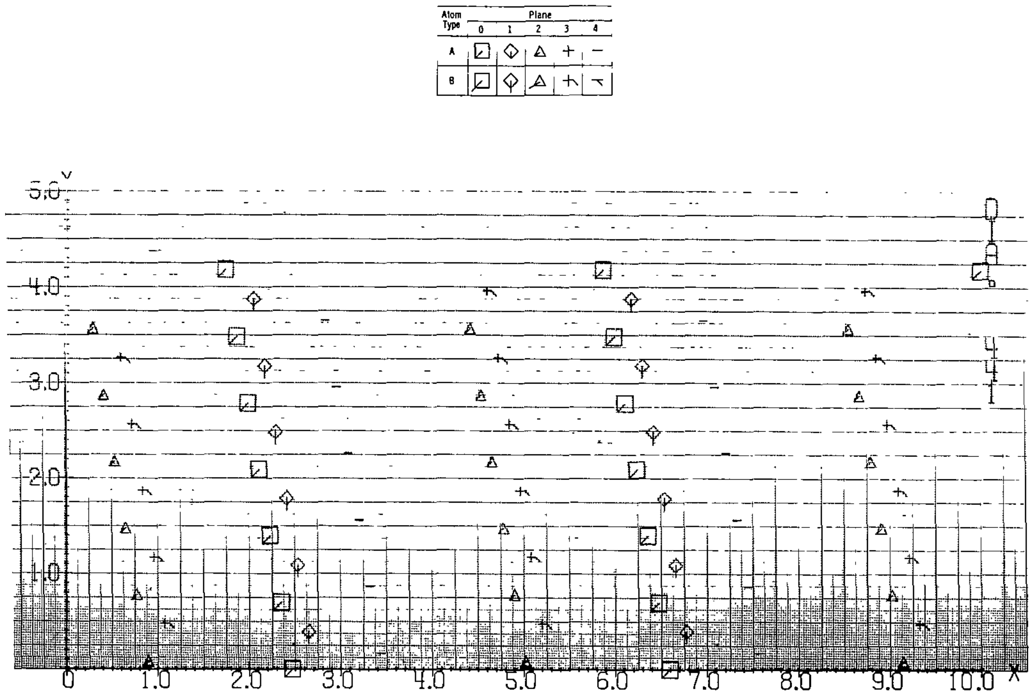


Figure 116. - Diamond structure; 441 plane.

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