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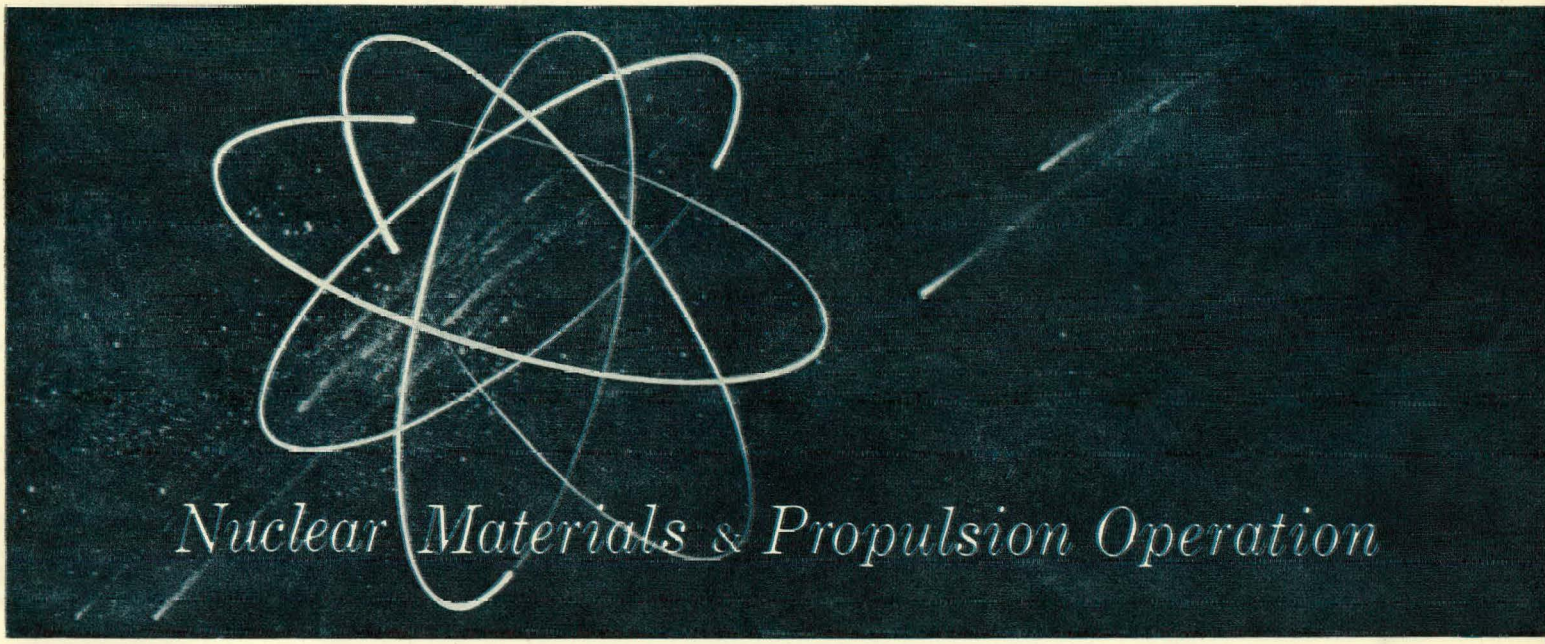

COMPUTER PROGRAMS DESCRIBING COLLISION CASCADES IN BINARY MATERIALS II. WURTZITE STRUCTURE

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ABSTRACT

An IBM 7090 computer program calculates the results of knock-on cascades initiated by the injection of a single atom into a binary solid. The program represents an extension to the real wurtzite structure of beryllium oxide, of an earlier calculation in which, for simplicity, the cascade was confined to a square planar lattice. Interactions between atoms are computed using a hard sphere approximation to the Bohr screened coulomb potential. Output from the computer includes a complete cascade history, including range and displacement statistics, and a listing of the final pattern of point defects. The program is designed to assist in interpreting the results of ion bombardment experiments on BeO.

I. INTRODUCTION

This report describes an IBM 7090 computer program which is the second in a series intended to describe the detailed features of knock-on cascades produced in binary solids by ion bombardment.

An earlier program [1] traced such cascades under the simplifying assumption of a square planar lattice (SPL). Using the experience gained in programming and in analyzing results from the SPL program, the present code was written, applying the same physical laws, but introducing the additional complexity of the real three-dimensional crystal structure of wurtzite.

The basic physical assumptions underlying the calculation are retained from the SPL program and consist of the following:

1) All interactions between atoms may be approximated by elastic collisions between two hard spheres, one of which is initially at rest. The sphere radius is taken to be the distance of closest approach implied by the Bohr screened coulomb potential.

2) The criterion for atom displacement is the model of Snyder and Neufeld. (See II.5).

The computer output consists of the straight-line distance travelled by the injected primary atom, the number of atoms of each type displaced in the cascade, a complete history of all collisions, if desired, and a table showing the final configuration of point defects.

Results which may be obtained from running the program include the following:

1) Pictures of the form taken by the collision cascade. These are obtained by plotting the projection onto various planes of the paths taken by the primary atom and the knock-ons.

2) The energy distribution of primary knock-ons and of all displaced atoms.

3) The range distribution of primary atoms with a specified energy.

4) The effect of crystal geometry on stopping power.

5) The displacement functions (g-functions) for primary knock-ons.

6) Three-dimensional pictures of the form taken by the pattern of damage in the crystal, and information about defect clustering. The pictures were obtained by plotting the information contained in the defect table on stacked plexiglass sheets, using map tacks inserted in perforations corresponding to the atom sites and interstices of the wurtzite structure.

These results will be useful in interpreting the results of ion bombardment experiments and in providing a basis for analytical work on the kinetics of annealing by giving a picture of the spatial distribution of simple defects and defect clusters.

In addition, the wurtzite program, as a first attempt to perform a meaningful three-dimensional radiation damage calculation using a real crystal structure, will provide the foundation for further calculations using more sophisticated collision laws and other crystal structures.

II. PHYSICAL MODEL AND COMPUTATION METHODS

1. General Problem

Given information about a wurtzite structure and a single primary atom moving in the structure, the task of the program is to locate all collisions in the cascade of activity resulting from the presence of the moving atom, and determine the results of these collisions, using the hard sphere collision laws. In particular, for each collision the energy transfer and scattering angle are computed, and a determination is made of which, if either, of the two atoms is free after the collision to move on through the lattice and have other collisions. This process continues until the entire amount of energy supplied by the primary has been dissipated by displacing atoms from their sites and by agitating them thermally.

The non-geometrical aspects of the wurtzite calculation are similar in many respects to those of the SPL calculations. Those items which are identical in the two programs are discussed only briefly in this report. Where necessary, reference is made to the SPL report for a more complete discussion.

2. The Wurtzite Structure

In connection with experiments on ion bombardment of beryllium oxide, the wurtzite crystal structure is of interest. Wurtzite is a hexagonal structure usually associated in the literature with zinc sulfide.

For the purposes of this calculation, it was convenient to impose a rectangular grid upon the crystal, dividing it into identical "boxes". See Fig. 1. The usual orthogonal x, y, and z axes are used, with the separation distance

FIGURE 1a - XY PLANE - LOWER

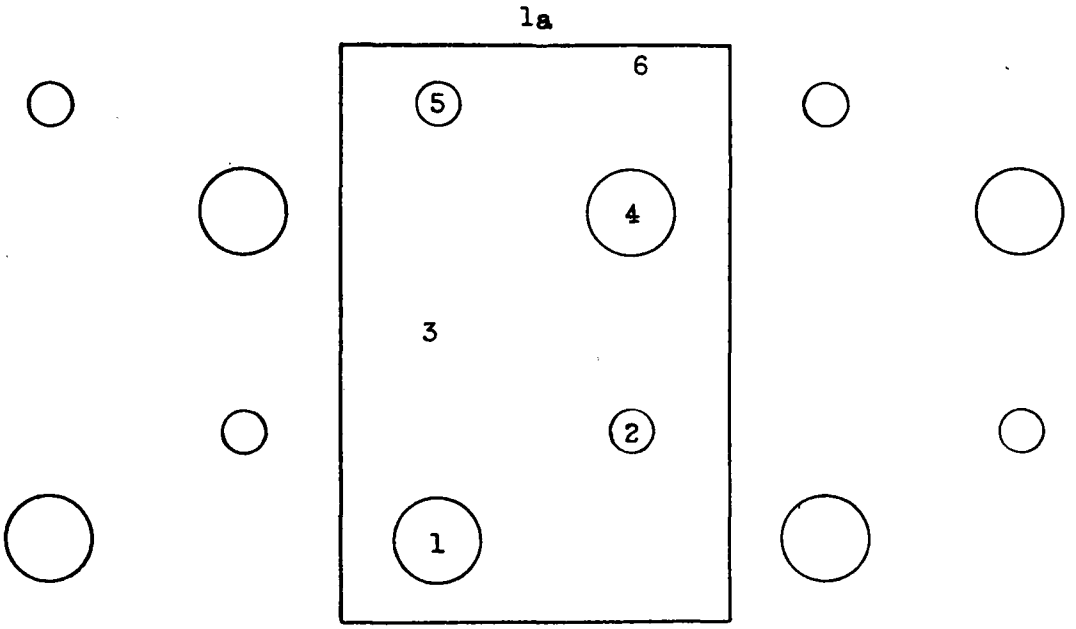

FIGURE 1b - XY PLANE - UPPER

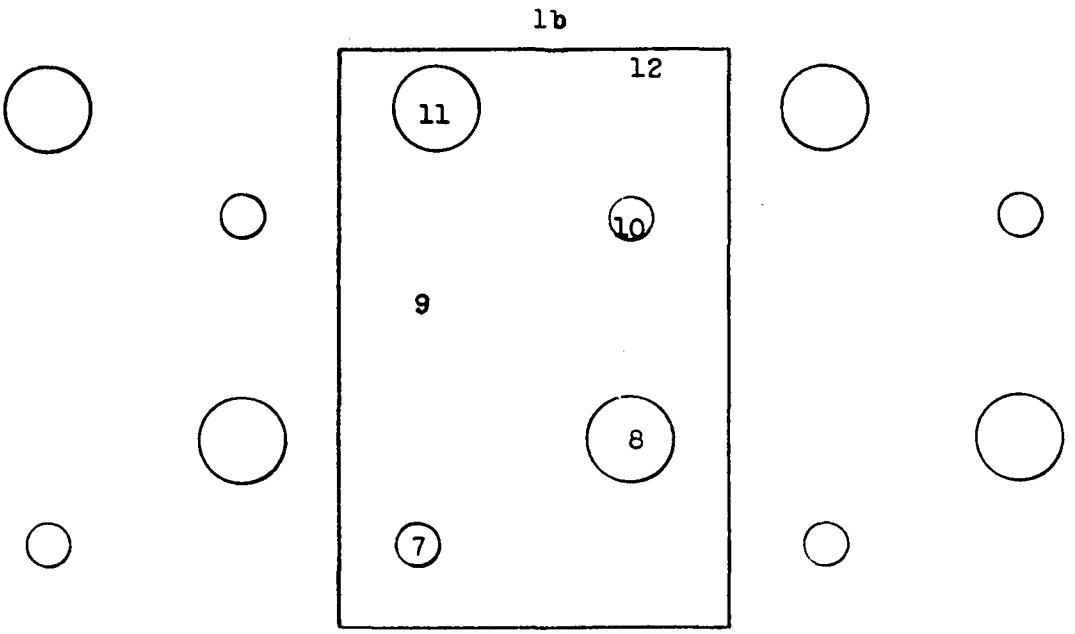

FIGURE 1c - XZ PLANE - FRONT

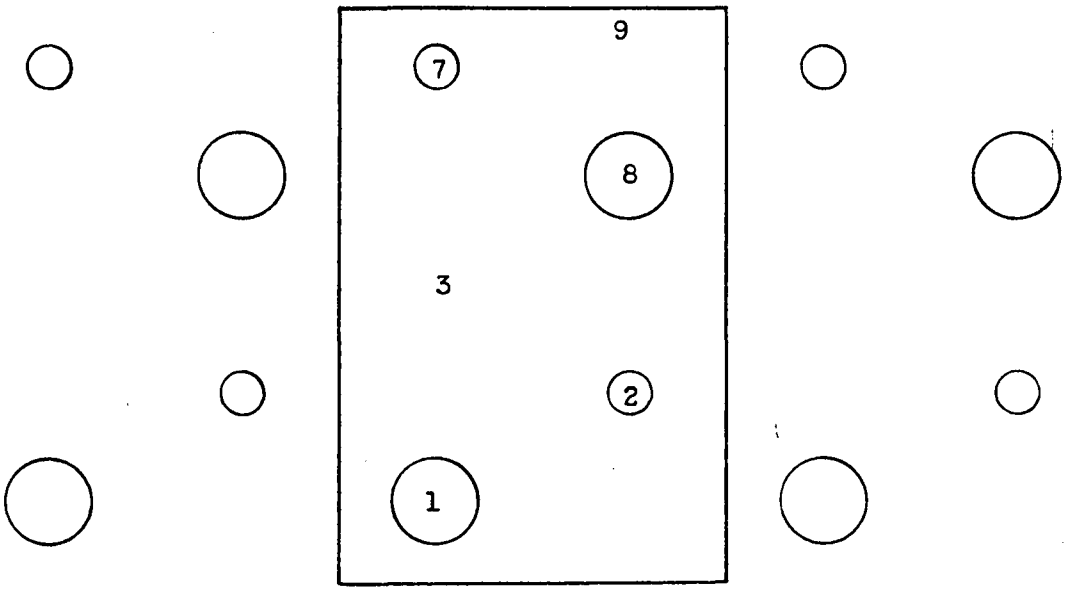

FIGURE 1d - XZ PLANE - REAR

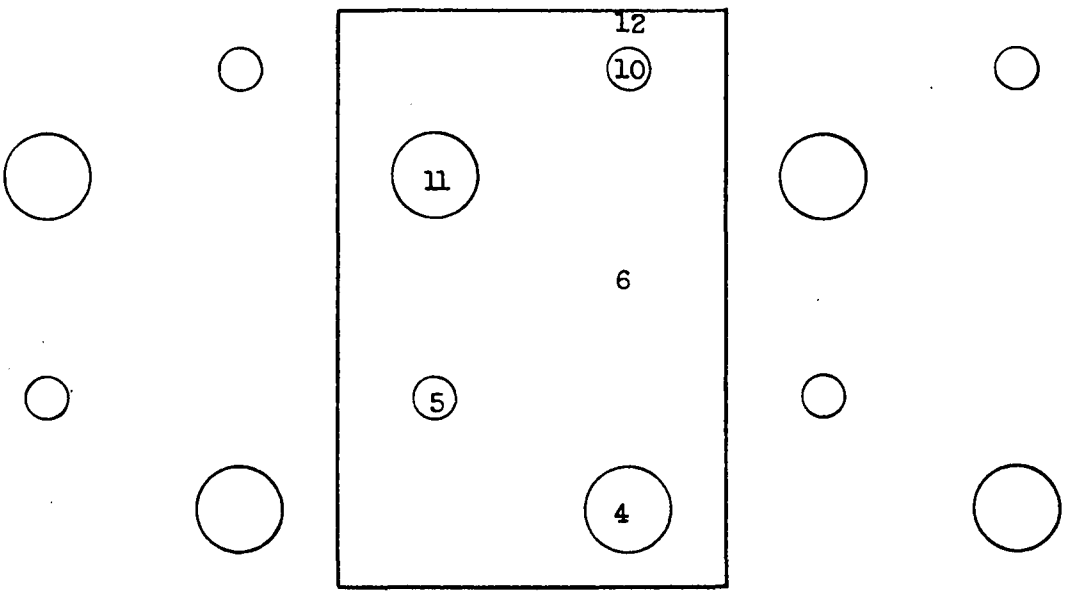

FIGURE 1. XY AND XZ PROJECTIONS OF WURTZITE LATTICE SITES AND INTERSTITIALS.

between grid planes dictated by the repetition of configurations along the three directions. In other words, the grid is chosen so that each box is identical with respect to the set of lattice sites it contains.

The dimensions of the lattice are described by the lattice constants a and c, where a is the separation distance between like atoms along the x-direction, and c is the separation distance between like atoms along the z-direction. Other constants of interest are A, the interatomic first neighbor distance, and B, the distance between close XY planes of unlike atoms.

$$(1) \qquad B = \sqrt{A^2 - \frac{a^2}{4 \cos^2 \pi/6}}$$

For room temperature beryllium oxide, these constants are: [2]

$$a = 2.69 \text{ Å}$$
$$c = 4.39 \text{ Å}$$
$$A = 1.65 \text{ Å}$$
$$B = 0.54 \text{ Å}$$

The computational elements of space are boxes (rectangular parallelipipeds) determined by the above-mentioned grid. A box has dimensions as follows:

$$(2) \qquad D_x = 2\sqrt{A^2 - B^2} \cos \pi/6$$

$$(3) \qquad D_y = 2\sqrt{A^2 - B^2} (1 + \sin \pi/6)$$

$$(4) \qquad D_z = 2 (A + B)$$

Each box contains twelve possible positions for atoms, eight normal atom sites and four interstitial positions. Specifically, the contents of a box are given by the following table, where (x_o, y_o, z_o) is the box origin.

Position Number (i)	x_i	y_i	z_i	Type Position
1	$x_o + 1/2\sqrt{A^2-B^2}\cos\pi/6$	$y_o + 1/4\sqrt{A^2-B^2}$	$z_o + A/4$	O
2	$x_1 + 3/2\sqrt{A^2-B^2}\cos\pi/6$	$y_1 + \sqrt{A^2-B^2}\sin\pi/6$	$z_1 + B$	B
3	x_1	$y_1 + 1/2\sqrt{A^2-B^2}$	$z_1 + A/2$	Int.
4	x_2	$y_3 + A/2$	z_1	O
5	x_1	$y_4 + \sqrt{A^2-B^2}\sin\pi/6$	z_2	B
6	x_2	$y_5 + 1/2\sqrt{A^2-B^2}$	z_3	Int.
7	x_1	y_1	$z_1 + A + 2B$	B
8	x_2	y_2	$z_2 + A$	O
9	x_3	y_3	$z_7 + A/2$	Int.
10	x_4	y_4	z_7	B
11	x_5	y_5	z_8	O
12	x_6	y_6	z_9	Int.

For illustrations of the wurtzite structure, see references [3], [4], and [5].

In addition to BeO, the wurtzite structure is also displayed by the following compounds and alloys [6]: Ag In S_2 (H.T.), AlN, $Al_2S_4Z_n$ (H.T.), Al_2Se_3, CdS, CdSe, Cr_2H to CrH, CrO (?), CuH (?), GaN, β-Ga_2S_3, InN, MgTe, β'-MnS, γ-MnSe, ZnO, ZnS.

3. Tracing Method

Given parameters describing an energetic atom (P_1) moving in the crystal, the first task of the computer is to search out the next atom for which the results of a collision are to be computed. Since only binary events are considered, only one atom need be chosen.

Assume P_1 to be located at (x_1, y_1, z_1) in box (i, j, k). The first set of atoms to be tested consists of those located in box (i, j, k). If the box contains interstitials, all positions are tested; if not, only positions 1, 2, 4, 5, 7, 8, 10, and 11 are tested.

In testing a position, the computer executes the following sequence:

1) Determines whether the position is that of one of the two most recent targets collided with by P_1. If so, the position is rejected. This test is made in order to prevent "cycling", i.e. repeated collisions alternatively with a pair of atoms between which P_1 is passing.

2) Looks up occupancy of the position. If vacant, it is rejected.

3) If occupied, computes the projection D_m of the line joining the centers of P_1 and the prospective target, along the line of flight of P_1,

$$(5) \quad D_m = (x_i - x_1) \cos \alpha + (y_i - y_1) \cos \beta + (z_i - z_1) \cos \gamma$$

where (x_i, y_i, z_i) is the position of the center of the prospective target and the cosines are direction cosines for P_1. If D_m is negative, the position is rejected. If D_m is not the smallest positive D_m computed so for any position in this box, the position is rejected.

4) Otherwise, the impact parameter for P_1 and this target is calculated.

$$(6) \quad p = [(x_i - x_1)^2 + (y_i - y_1)^2 + (z_i - z_1)^2 - D_m^2\ ]^{1/2}$$

If $p > p_{max}$, the position is rejected. p_{max} is an input quantity.

Thus, the atom at the position in the box for which the smallest positive D_m is computed, and is not rejected for other reasons, is taken to be the target (P_2).

If every atom in the box is rejected, a new box is selected and the process is repeated.

The selection of the next box proceeds according to the following scheme: x_B, y_B, and z_B are computed, where x_B is the x-coordinate of the next YZ grid plane (box boundary) to be pierced by the line of flight of P_1, y_B is the y-coordinate of the next XZ plane, and z_B is the z-coordinate of the next XY plane.

Three secondary boxes are thus determined. These boxes are ordered by arranging the quantities $| x_1 - x_B |$, $| y_1 - y_B |$, and $| z_1 - z_B |$ in ascending order, i.e., in order of "nearness". The three boxes are then tested in this order, to find an acceptable target, the rejection procedure being that described above.

4. Calculation of Scattering Angle and Energy Transfer

The following discussion assumes a moving atom (P_1) has been found to be in collision with a stationary target atom (P_2) located by the method of II.3. Subscripts 1 and 2 refer throughout to the moving and target atoms respectively.

a) Hard sphere radius

The two atoms are assumed to collide at the separation distance equal to the distance of closest approach associated with the potential V(r) appropriate to the collision process. This is defined to be the separation distance at which the radial velocity component vanishes [7].

$$(7)\quad \text{radial velocity} = \frac{dr}{dt} = \sqrt{\frac{2}{M_o}\left[E_o - V(r) - \frac{\ell^2}{2M_o r^2}\right]}$$

where r is the distance between centers, V is the potential energy at separation r, ℓ is the angular momentum of the collision, E_o is the total kinetic energy in the center of mass coordinate system, and M_o is the reduced mass of the system.

$$(8)\qquad M_o = \frac{M_1 M_2}{M_1 + M_2}$$

$$(9)\qquad \ell = p\sqrt{2\,M_o\,E_1} = \text{constant}$$

$$(10)\qquad E_o = E_1\,\frac{M_o}{M_1}, \quad \text{from which it follows that}$$

$$(11)\qquad \frac{\ell^2}{2M_o r^2} = \frac{p^2}{r^2}\left(\frac{M_o}{M_1}\right) E_1$$

Thus, from (7), dr/dt = 0 when

$$(12)\qquad V(r) = E_o - \frac{\ell^2}{2M_o r^2}$$

Inserting (10) and (11), (12) becomes,

$$(13) \qquad V(r) = \frac{M_o}{M_1} E_1 \left(1 - \frac{p^2}{r^2}\right)$$

The calculations assume the Bohr exponentially screened coulomb potential:

$$(14) \qquad V(r) = \frac{z_1 z_2 \exp(-r/a)}{r}$$

where

$$(15) \qquad a = \frac{\lambda a_h}{(z_1^{2/3} + z_2^{2/3})^{1/2}} = \text{screening radius}$$

$$(16) \qquad a_h = 0.529172 \text{ Å}$$

Combining (13) and (14) yields

$$(17) \qquad r = \frac{M_1 + M_2}{M_2} \frac{z_1 z_2}{E_1} \exp(-r/a) \left(1 - \frac{p^2}{r^2}\right)^{-1}$$

For each collision, the computer employs a Newton-Raphson iteration to solve (17), thus obtaining the distance of closest approach for the collision, which is the sphere radius to be used in computing the results of the collision using the hard sphere model.

The parameter λ is an input value which adjusts the "hardness" of the Bohr potential.

For larger values of p, ($p \geq 1$ Å), (17) may be approximated by

$$(18) \qquad r = p(1 + \epsilon)$$

where

$$(19) \qquad \epsilon = \frac{z_1 z_2 \left(\frac{M_1 + M_2}{M_2} \right) \exp(-r/a)}{p E_1}$$

In contrast, some investigators have employed a hard sphere approximation which is independent of impact parameter; i.e., the distance of closest approach is always calculated for a head-on (p = 0) collision [8].

The above scheme always results in a solution r such that r > p, in other words, a "miss" is not possible. This has the effect, in computation, that an atom cannot enter and remain in a region of zero potential, which would result in the computer hunting indefinitely for a collision.

b) Point of collision

Given atoms P_1 with center at (x_1, y_1, z_1) and P_2 with center at (x_2, y_2, z_2), in collision with hard sphere radius r, the method for computing the point of contact (x_c, y_c, z_c) is described below.

r is in reality an effective radius depending upon both P_1 and P_2. Geometrically, we assume P_1 has radius zero, and P_2 has radius r, so that

$$(20) \qquad r^2 = (x_c - x_2)^2 + (y_c - y_2)^2 + (z_c - z_2)^2$$

Expressing x_c, y_c, and z_c parametrically:

$$(21) \qquad x_c = x_1 + a_1 t$$

(22) $$y_c = y_1 + b_1 t$$

(23) $$z_c = z_1 + c_1 t$$

where a_1, b_1, and c_1 are the direction cosines for P_1.

Substituting (21), (22), and (23) in (20),

(24) $$(x_1 + a_1 t - x_2)^2 + (y_1 + b_1 t - y_2)^2 + (z_1 + c_1 t - z_2)^2 - r^2 = 0$$

Expanding (24) and collecting terms,

(25) $$(x_1 - x_2)^2 + 2 a_1 t (x_1 - x_2) + a_1^2 t_1^2 + (y_1 - y_2)^2 + 2 b_1 t (y_1 - y_2) + b_1^2 t_1^2 + (z_1 - z_2)^2 + 2 c_1 t (z_1 - z_2) + c_1^2 t^2 - r^2 = 0$$

Using the fact that $a_1^2 + b_1^2 + c_1^2 = 1$, (25) may be written as a quadratic in t:

(26) $$t^2 + 2 Bt + C = 0$$

where

(27) $$B = [a_1 (x_1 - x_2) + b_1 (y_1 - y_2) + c_1 (z_1 - z_2)]$$

$$(28) \qquad C = [\,(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2 - r^2\,]$$

The solutions to (26) are:

$$(29) \qquad t_1 = -B + \sqrt{B^2 - C}$$

$$(30) \qquad t_2 = -B - \sqrt{B^2 - C}$$

Letting T be minimum positive value of $\{ t_1, t_2 \}$, the solution for the point of collision follows from (21), (22), and (23):

$$(31) \qquad x_c = x_1 + a_1 T$$

$$(32) \qquad y_c = y_1 + b_1 T$$

$$(33) \qquad z_c = z_1 + c_1 T$$

c) Scattering angles (See Figure 2)

The direction cosines for the path of P_2 after collision are given by:

$$(34) \qquad a_2 = (x_2 - x_c)/r$$

$$(35) \qquad b_2 = (y_2 - y_c)/r$$

$$(36) \qquad c_2 = (z_2 - z_c)/r$$

Let (a_1', b_1', c_1') be the set of direction cosines for P_1 after collision. Taking the cross product of the vectors (a_1', b_1', c_1') and (a_1, b_1, c_1), we find that the vector with direction numbers

$$(37) \qquad a_u = b_1' c_1 - b_1 c_1'$$

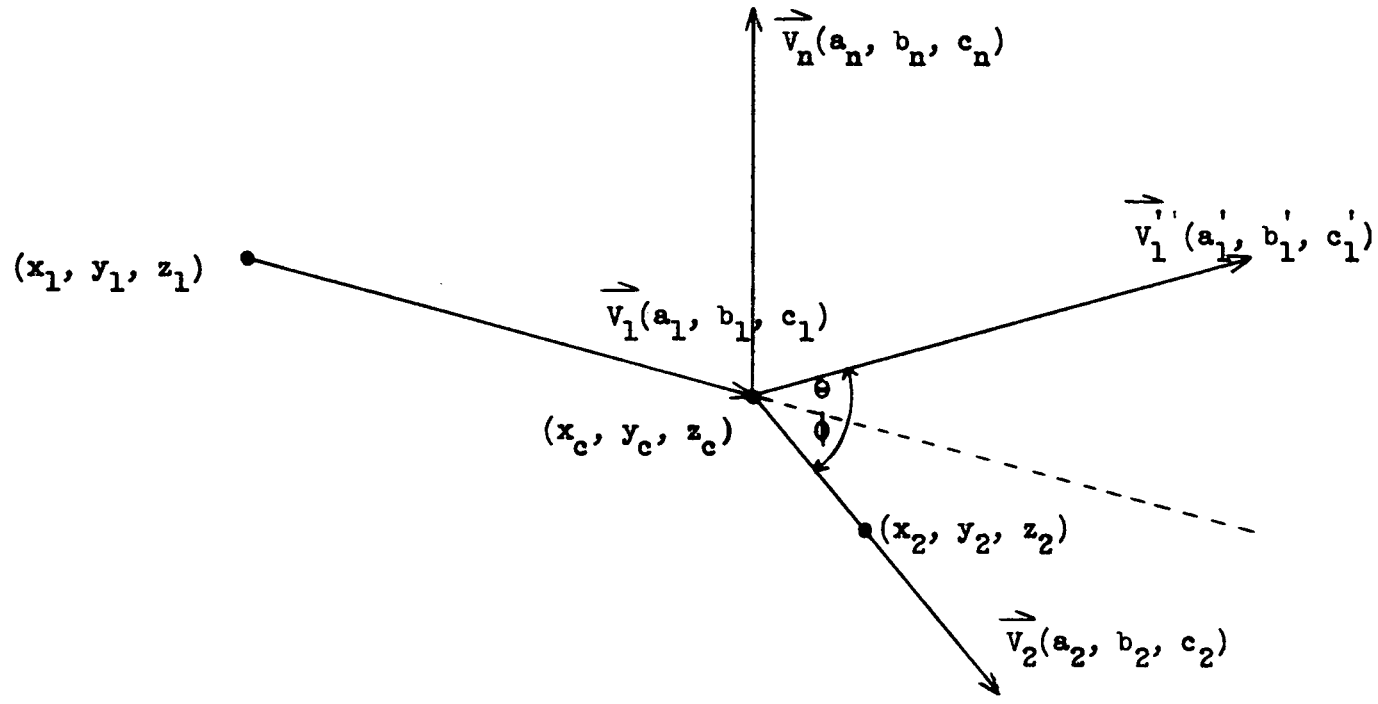

FIGURE 2

SCATTERING ANGLE CALCULATION

$$(38) \qquad b_n = c_1' a_1 - c_1 a_1'$$

$$(39) \qquad c_n = a_1' b' - a_1 b_1'$$

is normal to the collision plane.

Considering dot products involving (a_1', b_1', c_1'), we can now write three simultaneous linear equations in (a_1', b_1', c_1').

$$(40) \qquad a_n a_1' + b_n b_1' + c_n c_1' = 0$$

$$(41) \qquad a_2 a_1' + b_2 b_1' + c_2 c_1' = \cos(\theta + \varphi)$$

$$(42) \qquad a_1 a_1' + b_1 b_1' + c_1 c_1' = \cos\theta$$

where θ is the angle through which P_1 is scattered, and φ is the angle of P_2 relative to the original direction of P_1.

From the hard sphere model [1] we know that

$$(43) \qquad \sin\varphi = p/r$$

$$(44) \qquad \cos\theta = \frac{\frac{M_1}{M_2} + 2\sin^2\varphi - 1}{\left[\left(\frac{M_1}{M_2}\right)^2 + 2\,\frac{M_1}{M_2}\left(2\sin^2\varphi - 1\right) + 1\right]^{1/2}}$$

The equations (40), (41), and (42) are then solved in the usual fashion, yielding

$$(45) \qquad a_1' = \frac{D_1}{D}$$

$$(46) \qquad b_1' = \frac{D_2}{D}$$

$$(47) \qquad c_1' = \frac{D_3}{D}$$

where

$$(48) \qquad D = \begin{vmatrix} a_n & b_n & c_n \\ a_2 & b_2 & c_2 \\ a_1 & b_1 & c_1 \end{vmatrix}$$

$$(49) \qquad D_1 = \begin{vmatrix} 0 & b_n & c_n \\ \cos(\theta+\varphi) & b_2 & c_2 \\ \cos\theta & b_1 & c_1 \end{vmatrix}$$

$$(50) \qquad D_2 = \begin{vmatrix} a_n & 0 & c_n \\ a_2 & \cos(\theta+\varphi) & c_2 \\ a_1 & \cos\theta & c_1 \end{vmatrix}$$

$$(51) \qquad D_3 = \begin{vmatrix} a_n & b_n & 0 \\ a_2 & b_2 & \cos(\theta+\varphi) \\ a_1 & b_1 & \cos\theta \end{vmatrix}$$

d) Energy transfer

The energy transfer from P_1 to P_2 by the collision is given by [9].

$$(52) \qquad E_{TR} = \frac{4 M_1 M_2 E_1 \cos^2 \varphi}{(M_1 + M_2)^2}$$

5. Displacement Model

The model for atomic displacement which is assumed in the calculations is one due to Snyder and Neufeld [10]. The four types of collisions possible in this model are outlined in detail in [1] and illustrated schematically by Figure 3.

The differences between this model and two other well-known models [10] should be pointed out. The model of Kinchin and Pease differs in that the struck atom is not assumed to lose energy E_d before moving off through the lattice to possibly make other displacements. The model of Seitz and Harrison differs in that there is no allowance for the possibility of replacement collisions.

In a monatomic material, the number of displacements $\nu(E)$ predicted theoretically by the different models is as follows:

$$(53) \qquad \text{Seitz-Harrison:} \qquad \nu(E) \cong 0.561 \ (E/E_d)$$

$$(54) \qquad \text{Kinchin-Pease:} \qquad \nu(E) \cong 0.5 \ (E/E_d)$$

$$(55) \qquad \text{Synder-Neufeld:} \qquad \nu(E) \cong 0.35 \ (E/E_d)$$

6. Scheduling of Collision Traces

In general, the injection of an energetic atom into a lattice causes a heavily branching cascade of collisions. The computer must thus approximate

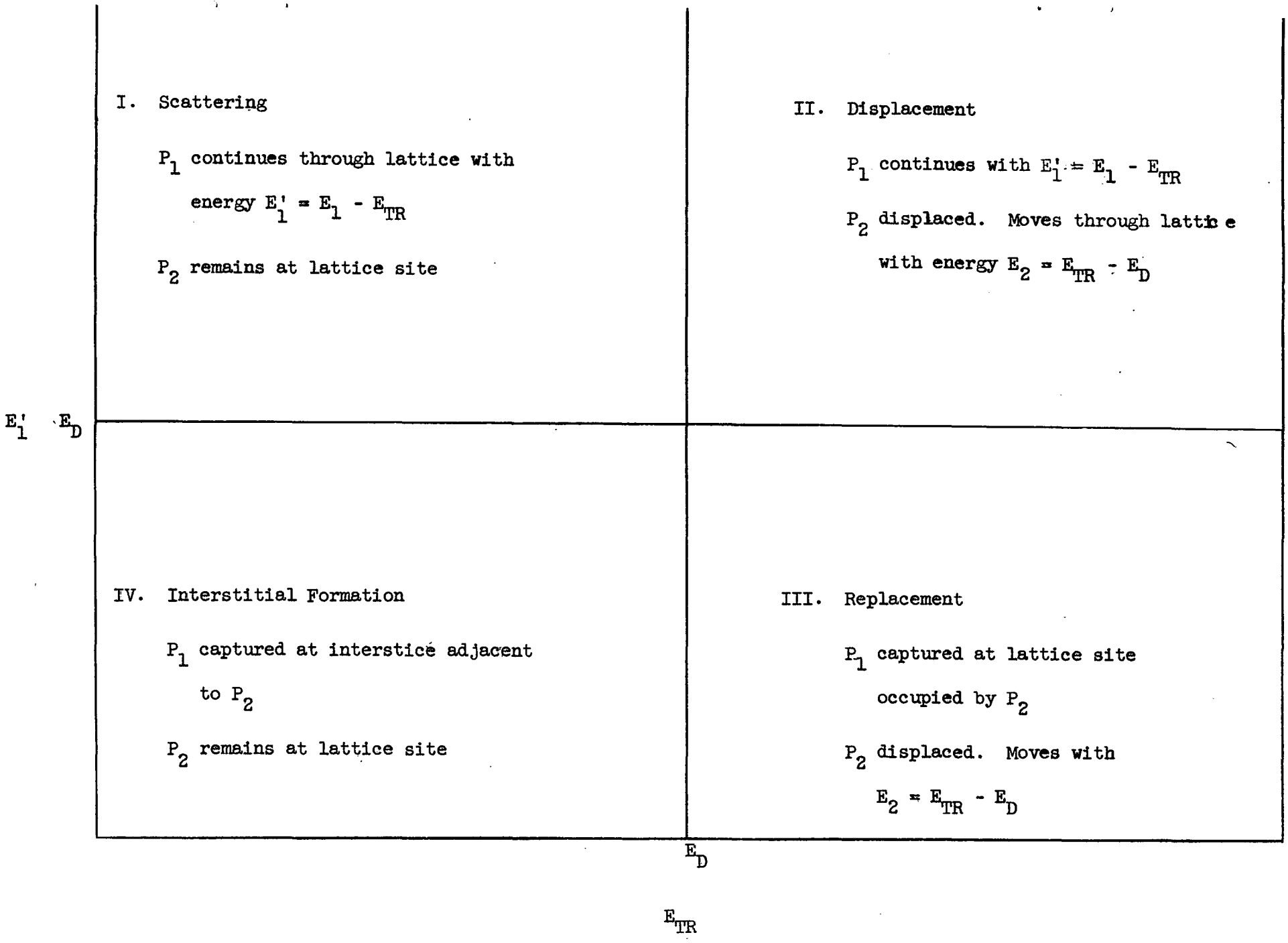

Fig. 3 - Snyder-Neufeld model for atom displacement.

a large number of events occurring more or less simultaneously by computing successively the results of separate, independent, binary collisions. The scheduling of these calculations is guided by the following two rules:

(1) Each atom in the set of atoms moving though the lattice at a given time is traced to its next collision before any atom in the set is traced a second time.

(2) When a displacement occurs, the post-collision velocities of the projectile and target atoms determine the order of tracing. The fastest one is traced first.

The computer keeps a table of the parameters describing each free atom. Section II.6 of [1] describes the handling of this table.

7. Placement of Interstitials

When a collision occurs in which P_1 fails to displace P_2, but is itself left with energy less than E_d, the program inserts P_1 into one of the neighboring interstices (box positions 3, 6, 9, 12). Which interstice is chosen depends upon the box position of P_2 and upon the location of the point of collision (x_c, y_c, z_c) relative to (x_i, y_i, z_i), the center of P_2. The "octant" of the sphere with center at (x_i, y_i, z_i) in which $(x_c\ y_c, z_c)$ lies is the determining factor. The nearest interstice to P_2 in the direction of the octant of collision is the one chosen.

The octants are numbered as follows:

Octant	$x_c - x_i$	$y_c - y_i$	$z_c - z_i$
1	+	+	+
2	-	+	+
3	-	-	+
4	+	-	+
5	+	+	-
6	-	+	-
7	-	-	-
8	+	-	-

The table below gives the interstices determined by P_2 and the octant of collision. Box (I) gives the coordinates of the box containing I relative to the coordinates of the box containing P_2, i.e. taking the coordinates of the latter to be (0, 0, 0).

Pos (P_2)	Octant	Pos(I)	Box(I) x	y	z
1	1	3	0	0	0
1	2	3	0	0	0
1	3	6	-1	-1	0
1	4	6	0	-1	0
1	5	9	0	0	-1
1	6	9	0	0	-1
1	7	12	-1	-1	-1
1	8	12	0	-1	-1

Pos (P_2)	Octant	Pos(I)	Box(I) x	y	z
2	1	3	1	0	0
2	2	3	0	0	0
2	3	6	0	-1	0
2	4	6	0	-1	0
2	5	9	1	0	-1
2	6	9	0	0	-1
2	7	12	0	-1	-1
2	8	12	0	-1	-1
4	1	6	0	0	0
4	2	6	0	0	0
4	3	3	0	0	0
4	4	3	1	0	0
4	5	12	0	0	-1
4	6	12	0	0	-1
4	7	9	0	0	-1
4	8	9	1	0	-1
5	1	6	0	0	0
5	2	6	-1	0	0
5	3	3	0	0	0
5	4	3	0	0	0
5	5	12	0	0	-1
5	6	12	-1	0	-1
5	7	9	0	0	-1
5	8	9	0	0	-1

Pos (P_2)	Octant	Pos(I)	Box (I) x	y	z
7	1	9	0	0	0
7	2	9	0	0	0
7	3	12	-1	-1	0
7	4	12	0	-1	0
7	5	3	0	0	0
7	6	3	0	0	0
7	7	6	-1	-1	0
7	8	6	0	-1	0
8	1	9	1	0	0
8	2	9	0	0	0
8	3	12	0	-1	0
8	4	12	0	-1	0
8	5	3	1	0	0
8	6	3	0	0	0
8	7	6	0	-1	0
8	8	6	0	-1	0
10	1	12	0	0	0
10	2	12	0	0	0
10	3	9	0	0	0
10	4	9	1	0	0
10	5	6	0	0	0
10	6	6	0	0	0
10	7	3	0	0	0
10	8	3	1	0	0

Pos (P_2)	Octant	Pos(I)	Box (I) x	y	z
11	1	12	0	0	0
11	2	12	-1	0	0
11	3	9	0	0	0
11	4	9	0	0	0
11	5	6	0	0	0
11	6	6	-1	0	0
11	7	3	0	0	0
11	8	3	0	0	0

If P_2 is itself an interstitial (position 3, 6, 9, or 12), that interstice is then recorded as having "multiple" occupancy and takes part in no further collision activity. This is a computational artifice having no physical basis. The situation occurs infrequently enough that it was not thought worthwhile to program a special procedure to handle it.

III. PROGRAM USAGE

1. Input

The input data is loaded by the variable field decimal input subroutine DING, and is punched in the usual DIP-DING format. See Appendix for example.

The following quantities are input data for the wurtzite program:

a) Lattice parameter

A Symbol: A

In angstroms. (See I.2). For room temperature BeO, A = 1.65 Å.

b) Lattice parameter

B Symbol: B

In angstroms. (See I.2). For room temperature BeO, B = 0.54Å.

c) Direction cosines

cos α	Symbols:	COSA
cos β		COSB
cos γ		COSG

Direction cosines for the initial path of the primary atom. An auxiliary Monte Carlo program has been written which will punch data cards for COSA, COSB, and COSG, randomized according to an isotropic distribution.

d) Primary energy

E Symbol: EO

Initial energy of the primary atom. (Electron volts)

e) Displacement energies

E_d Symbol: ED

ED(1) = threshold for displacement of a type 1 atom (Be) from a lattice site.

ED(2) = same for type 2. (O)

ED(3) = same for type 3. (Primary)

Units are electron volts.

f) Output control

Symbol: KPRINT

KPRINT(1) = 1: occupancy map suppressed

KPRINT(1) = 2: occupancy map printed

KPRINT(2) = 0: collision cascade history suppressed

KPRINT(2) = 1: collisions printed only for the primary atom

KPRINT(2) = 2: entire cascade printed

Both KPRINT(1) and KPRINT(2) are set equal to 2 at the beginning of each computer run and need not be included in the input unless a change is desired.

g) Charge

Z Symbol: PCHG

Nuclear charge (atomic number) for each of the three types of atoms. PCHG(K) = atomic number of type K atom.

h) Mass

M Symbol: PMASS

Mass number for each of the three types of atoms. PMASS(K) = mass of type K atom.

i) Maximum impact parameter

P_{max} Symbol: PMAX

Collisions with impact parameters greater than P_{max} will be ignored whenever a closer collision can be found in the original box or one of the three secondary boxes. Program results as a whole are not particularly sensitive to the choice of P_{max}. A value slightly less than the interatomic separation distance is reasonable. Entering a maximum radius speeds up the calculation by omitting the calculation of collision events with negligible effect. Units are centimeters.

j) Initial position of primary

x_o, y_o, z_o Symbols: XO, YO, ZO

Units are angstroms. The collision cascade is restricted to the "first octant", i.e., all coordinates positive. The crystal may be considered to have a "surface" consisting of the plane X = 0. If at any point in the cascade the X-coordinate of some atom becomes negative, it is recorded as having been "sputtered" from the surface. If a Y or Z coordinate becomes negative the program will malfunction. The initial position must be placed deep enough into the first octant to prevent this latter from happening, considering the initial direction which is given.

k) Bohr potential parameter

λ Symbol: XLMDA

Constant for use in computing screening radius (equation 15). In general, $1 \leq \lambda \leq 2$. The magnitude of the repulsive potential increases with increasing λ.

l) Atom names

Symbols: TYPE1, TYPE2, TYPE3

Each symbol is 2 machine words, consisting of the BCD name of the type 1, type 2, and primary atoms, respectively.

m) Option control to trace only the primary atom

Symbol: KPRIM

When KPRIM = 1, the secondary collision cascade is ignored by the computer, and only the history of the primary atom is traced. This is desirable when the object of the run is solely to obtain range statistics. The normal setting is KPRIM = 2, which is done by the program at the beginning of each run.

n) Change cases

Any number of histories may be calculated in one pass on the computer. Cases are separated by ends-of-record. For each history, only those data items need be changed which differ from the previous history.

2. Output (See Appendix for example)

a) Input printout

The first page of output for each history consists of the input parameters for the crystal and the primary atom.

b) Collision history

If KPRINT(1) = 2, a complete history of the knock-on cascade is printed out as it is computed. The columns are headed as follows:

N sequential number of collision.

TI type of incident atom.

TT type of target atom.

BOX box coprdinates (x, y, z) of the box containing P_2.

POS lattice position of P_2 within that box.
(See II.2 and Figure 1)

PBT spatial coordinates of the center of P_2 before collision (x_2, y_2, z_2)
(angstroms)

CPT spatial coordinates of the collision point. (x_c, y_c, z_c)

EBI energy of P_1 before collision (E_1) (electron volts).

EAI energy of P_1 after collision (E_1')

DBI direction cosines of P_1 before collision

DAI direction cosines of P_1 after collision

DAT direction cosines of P_2 after collision

ETR energy transferred from P_1 to P_2 by the collision

IPR impact parameter (angstroms)

RAD hard sphere radius

c) Occupancy table

If KPRINT(2) = 2, a table is printed at the end of the calculation giving the occupancy of all interstices and lattice sites in the region of the crystal affected by the cascade.

Five boxes are printed per line. The coordinates printed at the extreme left are the box coordinates of the first box of the line. The succeeding boxes on the same line have the same X and Y coordinates as the first box, but successively increasing Z-coordinates.

The columns of the printout represent box positions, referred to by number (positions 10, 11, and 12 are headed by X, Y, and Z, respectively).

Sites which retain their normal (undamaged) occupancy are left blank. Non-blank symbols are:

B	type 1 atom
O	type 2 atom

I	primary atom
V	vacancy
M	multiple interstitial

For example:

			1	2	3	4	5	6	7	8	9	X	Y	Z
100	100	100	V		I						B	O		

This is interpreted to mean that the primary atom has come to rest at position 3 of box (100, 100, 100). The oxygen atom at position 1 of this box has been displaced, leaving a vacancy. The beryllium atom at position 10 has been replaced by an oxygen atom. A beryllium atom has come to rest as an interstitial in position 9. Interstices 6 and 12 remain unoccupied. Sites 2, 4, 5, 7, 8, and 11 retain their normal occupancy.

d) Cascade and range statistics

The number of vacancies created during the cascade is printed, together with the number of interstitials of each type.

The penetration distance is printed (in angstroms). This is defined to be the straight line distance between (x_o, y_o, z_o) and the absorption point of the primary.

3. Running Time

In production runs to date, the program has computed at an average rate of approximately 40,000 collisions/hour, including the time required to print out the results of each collision. Omitting the collision printout increases the computing rate substantially, probably to about 60,000 collisions/hour.

However, the running time for a given history is somewhat uncertain because of the unpredictability of the number of collisions which will occur. A typical 50 keV cascade, for example, consists of 3000-3500 collisions. But it is not uncommon for atoms to become "channeled", i.e., travel for very long distances along certain crystallographic directions of low stopping power. Between 10,000 and 20,000 collisions might be computed for such an atom before it loses all its energy. So the possibility of anomalously long histories should be anticipated in estimating running time.

One should be judicious in requesting collision history printout. Since only 22 collisions can be printed on each page, a large group of high-energy runs can rapidly produce an awesome stack of paper. In addition, it slows down the calculation, as noted above.

4. Error Returns

DING performs the usual checking for input errors. The program itself checks the input after the first case has been read in. The message: "THE INPUT DATA IS BOTCHED UP -- TRY AGAIN", means that some necessary item has been omitted from the input data for the first case.

For checkout purposes, various subprograms call ERROR when impossible situations arise. By definition, impossible situations do not arise during production runs.

IV. PROGRAMMING INFORMATION

1. System and Setup

The wurtzite program is coded in FORTRAN and FAP for the IBM 7090. It

consists of a main program and 18 subroutines. No auxiliary tapes are required beyond the standard input and output tapes. The relocatable binary deck is loaded via the FORTRAN - FAP monitor.

The functions performed by the various subprograms are briefly described in the following section. See Fig. 4 for flow chart.

2. Subroutines

START: Initialization routine. Called at beginning of each machine run.

ICHEK: Checks for omissions in input data at the beginning of each run.

RESET: Initialization routine. Called after each new data record is read.

NEWBOX: Computes spatial coordinates of the sites in a given box.

SETUP: (Coded in FAP) Sets up occupancy record for the box, and keeps the occupancy record table for the entire crystal.

WRITE1: Prints out the input data.

SELECT: Given parameters describing a projectile atom, determines the site of the next collision.

OCCUP: (Coded in FAP) Interrogates the occupancy record of a box to determine the occupancy of a given site.

HSPHER: Hard sphere collision routine. Using the hard-sphere approximation, computes the trigonometric functions of the planar scattering angles, and from these the post-collision direction of both particles, and the energy transfer.

RADIUS: Routine to obtain hard sphere radius by solving equation for distance of closest approach.

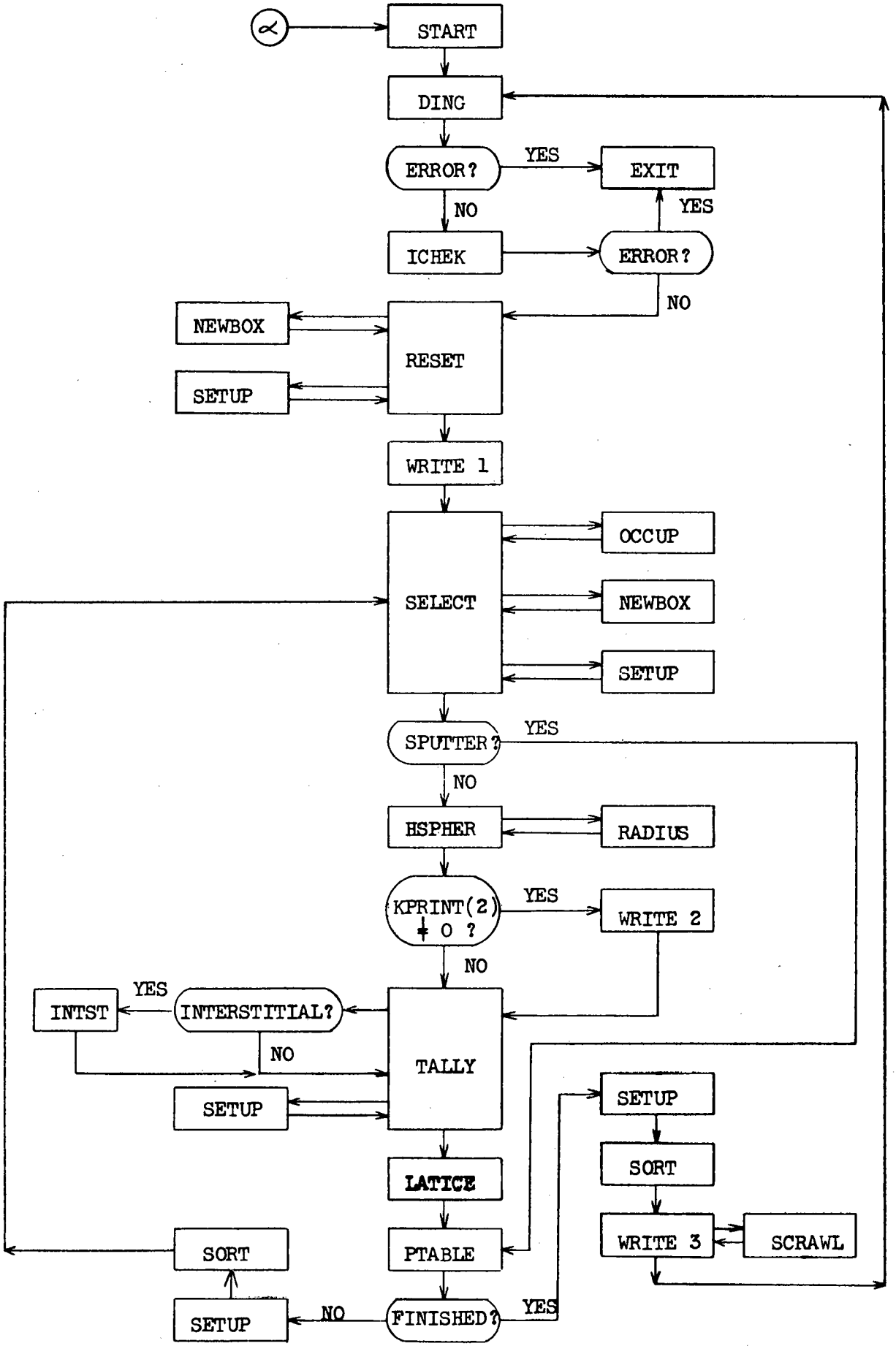

FIGURE 4

FLOW CHART

WRITE2: Prints out the collision history, if requested.

TALLY: Keeps running total of damage statistics. Classifies collision according to type.

INTST: (Coded in FAP) When the program determines that an interstitial is formed, INTST locates which interstice is to be filled, according to the scheme of section II.7.

SORT: Sorts the occupancy table into order prior to printing.

LATICE: (Coded in FAP) Updates the occupancy record after each collision.

PTABLE: Updates tables which contain parameters describing the atoms remaining to be traced.

SCRAWL: (Coded in FAP) Converts the internal occupancy record into BCD images for printing.

WRITE3: Prints the damage statistics, the range, and, if requested, the occupancy map.

3. Occupancy Table

What follows is a brief description of the manner in which information about the occupancy of the sites and interstices of the wurtzite lattice is handled internally by the computer.

The occupancy of each "box" (as defined in II.2) is described by one machine word. The 36 bits of the word are taken to be 12 octal digits, representing positions 1 through 12 of the crystal. The occupancy codes are the following:

0 - vacant

1 - type 1

2 - type 2

3 - primary

4 - "multiple"

A normal (i.e. undamaged) box would be represented by the occupancy code: 210210210210.

In order to conserve storage, occupancy codes are created only for those boxes which are actually affected by the cascade in the sense that it becomes necessary to search for a collision in the given box. The boxes are built up as needed as the cascade progresses. Thus core storage is not consumed in recording occupancy for extraneous parts of the lattice.

For the I-th box created (chronologically) in the course of the cascade, the three integers representing X, Y, and Z box coordinates are packed into KBOX(I).

The twelve octal digits making up the occupancy code are stored in BOX(I). This gives the computer access to the up-to-date occupancy of any site at any time during the cascade. The table is updated after each collision.

The occupancy table which is printed out at the end of the cascade is formed by comparing the occupancy of each box with normal occupancy and transforming the codes into appropriate BCD images by means of the 7090 convert instructions.

V. APPENDIX

1. Sample Input

2. Sample Output

Sample Input

Col. 1	2
	A, 1.65,
	B, 0.54,
	COSA, .55029, COSB, .33629, COSG, .76429,
	EO, 1000,
	ED, 25, 50, 100,
	PCHG, 4,8, 36,
	PMASS, 9, 16, 84,
	PMAX, 1.4/-8,
	XO, 270.73, YO, 469.71, ZO, 438.00,
	XLMDA, 1,
5	TYPE1, 2, BERYLLIUM
5	TYPE2, 2, OXYGEN
5	TYPE3, 2, KRYPTON
=	
8	

```
THREE-DIMENSIONAL ION BOMBARDMENT -- WURTZITE CRYSTAL

    TYPE 1 PARTICLE IS  BERYLLIUM      ATOMIC MASS =  9.
    TYPE 2 PARTICLE IS  OXYGEN         ATOMIC MASS = 16.

    INCIDENT PARTICLE IS  KRYPTON        ATOMIC MASS = 84.

    INITIAL ENERGY =  1000.0 (ELECTRON VOLTS)

    INITIAL COORDINATES (ANGSTROMS)

        X =  270.73000
        Y =  469.71000
        Z =  438.00000

    INITIAL DIRECTION COSINES

        COS ALPHA =0.55029
        COS BETA =0.33629
        COS GAMMA =0.76429

    DISPLACEMENT ENERGIES

        BERYLLIUM      25.0 EV
        OXYGEN         50.0 EV

    LATTICE PARAMETERS (ANGSTROMS)
        A=  1.65  B=  0.54
```

COLLISION HISTORY

NO	TI	TT	BOX	POS	PBT	CPT	EBI	EAI	DBI	DAI	DAT	ETR	IPR	RAD
1	3	1	100	2	272.08	271.37	1000.00	999.63	0.55029	0.54718	0.51232	0.37	1.3856	1.3863
			100		468.91	470.10			0.33629	0.34170	-0.85729			
			100		438.95	438.88			0.76429	0.76409	0.05077			
2	3	1	100	5	270.73	271.40	999.63	999.16	0.54718	0.55085	-0.49779	0.47	1.3533	1.3543
			100		471.29	470.12			0.34170	0.33561	0.86713			
			100		438.95	438.93			0.76409	0.76416	0.01677			
3	3	2	100	4	272.08	271.37	999.16	984.23	0.55085	0.51506	0.74327	14.93	0.9319	0.9452
			100		470.51	470.10			0.33561	0.31478	0.43468			
			100		438.41	438.89			0.76416	0.79726	-0.50853			
4	3	1	100	2	272.08	271.37	984.23	983.86	0.51506	0.51192	0.51104	0.37	1.3860	1.3867
			100		468.91	470.10			0.31478	0.32027	-0.85812			
			100		438.95	438.88			0.79726	0.79710	0.04965			
5	3	1	100	5	270.73	271.40	983.86	983.39	0.51192	0.51560	-0.49607	0.47	1.3530	1.3539
			100		471.29	470.12			0.32027	0.31411	0.86813			
			100		438.95	438.93			0.79710	0.79717	0.01630			
6	3	2	100	4	272.08	271.35	983.39	969.26	0.51560	0.47909	0.76405	14.13	0.9390	0.9518
			100		470.51	470.09			0.31411	0.29284	0.44697			
			100		438.41	438.86			0.79717	0.82748	-0.46523			
7	3	1	100	2	272.08	271.37	969.26	968.90	0.47909	0.47592	0.51121	0.37	1.3862	1.3870
			100		468.91	470.10			0.29284	0.29836	-0.85814			
			100		438.95	438.89			0.82748	0.82733	0.04747			
8	3	1	100	5	270.73	271.39	968.90	968.42	0.47592	0.47961	-0.49300	0.47	1.3527	1.3536
			100		471.29	470.12			0.29836	0.29213	0.86990			
			100		438.95	438.93			0.82733	0.82743	0.01510			
9	3	2	100	4	272.08	271.33	968.42	955.03	0.47961	0.44250	0.78270	13.39	0.9458	0.9582
			100		470.51	470.08			0.29213	0.27051	0.45793			
			100		438.41	438.82			0.82743	0.85500	-0.42152			
10	3	1	100	2	272.08	271.36	955.03	954.67	0.44250	0.43930	0.51288	0.37	1.3865	1.3873
			100		468.91	470.10			0.27051	0.27605	-0.85731			
			100		438.95	438.89			0.85500	0.85487	0.04452			
11	3	1	100	5	270.73	271.39	954.67	954.19	0.43930	0.44298	-0.48852	0.47	1.3524	1.3534
			100		471.29	470.11			0.27605	0.26975	0.87245			
			100		438.95	438.93			0.85487	0.85499	0.01344			
12	3	1	100	10	272.08	272.22	954.19	801.80	0.44298	0.51543	-0.22550	152.40	0.4639	0.6294
			100		470.51	470.62			0.26975	0.31804	-0.16659			
			100		441.14	440.54			0.85499	0.79573	0.95989			
13	1	2	100	4	272.08	271.81	127.40	74.71	-0.22550	-0.76716	0.42219	52.68	0.4626	0.6230
			100		470.51	470.32			-0.16659	-0.56674	0.31189			
			101		442.79	442.26			0.95989	0.30045	0.85116			
14	3	2	101	11	273.43	272.61	801.80	796.23	0.51543	0.48950	0.75988	5.56	1.0630	1.0699
			100		471.29	470.86			0.31804	0.30446	0.40264			
			100		440.60	441.15			0.79573	0.81712	-0.51035			
15	1	2	100	1	270.73	270.27	74.71	72.19	-0.76716	-0.88009	0.40032	2.52	1.1250	1.1462
			100		468.13	469.18			-0.56674	-0.34896	-0.91403			
			101		442.79	442.87			0.30045	0.32197	-0.06558			
16	2	1	100	2	272.08	271.85	2.68	2.50	0.42219	0.41189	0.12578	0.19	1.6925	1.7602
			100		468.91	470.35			0.31189	0.49122	-0.81864			
			101		443.33	442.35			0.85116	0.76749	0.56036			
17	3	1	101	10	274.78	273.07	796.23	796.23	0.48950	0.48884	0.86207	0.00	1.9756	1.9756
			100		470.51	471.15			0.30446	0.30471	-0.32139			
			100		441.14	441.92			0.81712	0.81743	-0.39184			
18	1	1	99	2	269.37	269.85	72.19	5.59	-0.88009	-0.32236	-0.82289	66.61	0.1622	0.5831
			100		468.91	469.01			-0.34896	-0.63335	-0.17986			
			101		443.33	443.02			0.32197	-0.70353	0.53897			
19	3	1	101	5	273.43	273.54	796.23	683.18	0.48884	0.55012	-0.16801	113.05	0.5123	0.6647
			100		471.29	471.44			0.30471	0.35800	-0.21809			
			101		443.33	442.69			0.81743	0.75446	0.96136			
20	1	2	99	8	269.37	268.78	41.61	41.03	-0.82289	-0.89535	0.42159	0.58	1.3898	1.4004
			100		468.91	468.78			-0.17986	-0.19570	0.09215			

			101		444.98	443.72			0.53897	0.40007	0.90209				
21	1	2	101	11	273.43	273.24	88.05	45.68	-0.16801	-0.59815	0.28414	42.37	0.4542	0.6571	
			100		471.29	471.05			-0.21809	-0.77648	0.36885				
			101		444.98	444.40			0.96136	0.19824	0.88499				
22	3	2	101	1	273.43	273.78	683.18	682.23	0.55012	0.55496	-0.27489	0.94	1.2816	1.2832	
			101		472.81	471.60			0.35800	0.34291	0.94439				
			101		442.79	443.02			0.75446	0.75791	-0.18047				
23	3	2	101	8	274.78	275.24	682.23	680.09	0.55496	0.56539	-0.39042	2.14	1.1805	1.1840	
			101		473.59	472.50			0.34291	0.32093	0.92016				
			101		444.98	445.02			0.75791	0.75983	-0.02972				
24	3	1	102	7	276.13	275.52	680.09	540.50	0.56539	0.47606	0.95065	139.60	0.4111	0.6398	
			101		472.81	472.66			0.32093	0.32072	0.23613				
			101		445.52	445.39			0.75983	0.81884	0.20129				
25	1	2	102	8	277.48	277.19	114.60	108.10	0.95065	0.88199	0.29617	6.50	0.9358	0.9659	
			101		473.59	473.07			0.23613	0.06877	0.53341				
			101		444.98	445.75			0.20129	0.46623	-0.79231				
26	3	2	102	1	276.13	276.17	540.50	438.77	0.47606	0.54106	-0.06037	101.73	0.5800	0.7195	
			101		472.81	473.10			0.32072	0.44007	-0.40019				
			102		447.17	446.51			0.81884	0.71665	0.91444				
27	1	1	103	7	278.83	278.14	108.10	102.58	0.88199	0.75541	0.64680	5.51	1.0275	1.0548	
			101		472.81	473.15			0.06877	0.14504	-0.32111				
			101		445.52	446.25			0.46623	0.63899	-0.69176				
28	3	1	102	2	277.48	276.85	438.77	351.67	0.54106	0.45772	0.90019	87.10	0.4574	0.6958	
			101		473.59	473.65			0.44007	0.50603	-0.08885				
			102		447.71	447.42			0.71665	0.73105	0.42634				
29	2	1	102	7	276.13	276.00	51.73	46.96	-0.06037	-0.08975	0.11030	4.77	1.1049	1.1647	
			101		472.81	471.96			-0.40019	-0.59488	0.73111				
			102		449.90	449.12			0.91444	0.79879	0.67329				
30	1	2	103	8	280.18	278.73	102.58	102.58	0.75541	0.75004	0.62836	0.00	2.3057	2.3058	
			101		473.59	473.26			0.14504	0.14383	0.14260				
			101		444.98	446.75			0.63899	0.64556	-0.76474				
31	1	2	103	1	278.83	278.26	62.10	60.97	0.90019	0.82880	0.43925	1.13	1.2690	1.2817	
			101		472.81	473.51			-0.08885	0.00966	-0.54758				
			102		447.17	448.09			0.42634	0.55946	-0.71219				
32	3	2	102	8	277.48	277.56	351.67	349.35	0.45772	0.46172	-0.06985	2.32	1.1697	1.1770	
			101		473.59	474.43			0.50603	0.53327	-0.71809				
			102		449.36	448.55			0.73105	0.70883	0.69244				
33	2	2	102	11	276.13	276.01	46.96	13.51	-0.08975	-0.40561	0.15150	33.44	0.4257	0.7934	
			100		471.29	472.01			-0.59488	0.31268	-0.90367				
			102		449.36	449.04			0.79879	0.85890	0.40053				
34	1	2	103	1	278.83	278.63	102.58	69.36	0.75004	0.65417	0.27957	33.22	0.5603	0.6957	
			101		472.81	473.24			0.14383	0.74834	-0.62145				
			102		447.17	446.66			0.64556	0.10975	0.73187				
35	1	1	103	2	280.18	279.26	60.97	60.03	0.82880	0.75296	0.65719	0.94	1.3810	1.3918	
			101		473.59	473.52			0.00966	0.00379	0.04747				
			102		447.71	448.76			0.55946	0.65806	-0.75223				
36	3	1	102	10	277.48	278.01	349.35	330.42	0.46172	0.52228	-0.60637	18.93	0.8107	0.8820	
			101		475.19	474.95			0.53327	0.52731	0.26836				
			102		449.90	449.24			0.70883	0.67020	0.74853				
37	1	1	103	2	280.18	279.42	69.36	67.95	0.65417	0.57741	0.57964	1.41	1.2992	1.3126	
			101		473.59	474.14			0.74834	0.81639	-0.41866				
			102		447.71	446.79			0.10975	0.01016	0.69910				
38	1	1	103	7	278.83	279.44	60.03	58.94	0.75296	0.82103	-0.45063	1.09	1.3519	1.3643	
			101		472.81	473.52			0.00379	0.07490	-0.52362				
			102		449.90	448.92			0.65806	0.56596	0.72302				
39	3	2	103	11	278.83	278.37	330.42	301.22	0.52228	0.47567	0.52499	29.19	0.7910	0.8653	
			101		475.97	475.32			0.52731	0.44996	0.75301				
			102		449.36	449.71			0.67020	0.75583	-0.39669				
40	1	2	103	4	280.18	279.86	67.95	24.78	0.57741	0.09191	0.49110	43.17	0.3646	0.6542	
			101		475.19	474.76			0.81639	0.18582	0.66261				
			102		447.17	446.80			0.01016	-0.97828	0.56548				
41	1	2	103	8	280.18	279.64	58.94	4.97	0.82103	-0.96832	0.86396	53.97	0.0498	0.6193	
			101		473.59	473.54			0.07490	-0.07476	0.07572				
			102		449.36	449.05			0.56596	-0.23827	0.49784				
42	3	2	103	4	280.18	279.38	301.22	300.73	0.47567	0.46580	0.58262	0.49	1.3631	1.3652	
			101		475.19	476.27			0.44996	0.46429	-0.79298				

			103		451.55	451.31			0.75583	0.75330	0.17816					
43	2	1	104	7	281.53	280.58	3.97	2.14	0.86396	0.66598	0.73649	1.83	0.9100	1.2879		
			101		472.81	473.62			0.07572	0.54243	-0.63261					
			102		449.90	449.59			0.49784	0.51209	0.23956					
44	3	1	103	5	278.83	279.35	300.73	294.41	0.46580	0.49560	-0.51727	6.32	0.9883	1.0194		
			101		475.97	476.25			0.46429	0.48222	-0.27029					
			103		452.09	451.26			0.75330	0.72239	0.81202					
45	3	2	103	1	278.83	279.57	294.41	293.33	0.49560	0.51208	-0.58703	1.08	1.2643	1.2686		
			102		477.48	476.46			0.48222	0.46165	0.80924					
			103		451.55	451.58			0.72239	0.72433	-0.02297					
46	3	1	103	2	280.18	280.28	293.33	292.40	0.51208	0.51446	-0.08487	0.93	1.2641	1.2699		
			102		478.26	477.10			0.46165	0.44547	0.91594					
			103		452.09	452.59			0.72433	0.73273	-0.39224					
47	3	2	103	8	280.18	280.84	292.40	284.28	0.51446	0.56960	-0.64897	8.11	0.9919	1.0185		
			102		478.26	477.58			0.44547	0.40226	0.67167					
			103		453.74	453.38			0.73273	0.71676	0.35735					
48	3	1	104	7	281.53	281.10	284.28	235.32	0.56960	0.54325	0.55459	48.97	0.5450	0.7652		
			102		477.48	477.77			0.40226	0.49726	-0.36919					
			103		454.28	453.71			0.71676	0.67647	0.74574					
49	3	2	104	8	282.88	281.73	235.32	234.86	0.54325	0.52761	0.83754	0.46	1.3710	1.3735		
			102		478.26	478.34			0.49726	0.49880	-0.05417					
			103		453.74	454.49			0.67647	0.68762	-0.54369					
50	1	2	104	1	281.53	281.98	23.97	21.25	0.55459	0.77347	-0.38669	2.72	1.0993	1.1739		
			102		477.48	477.18			-0.36919	-0.51491	0.25743					
			104		455.93	454.89			0.74574	0.36960	0.88555					
51	3	1	104	2	282.88	282.67	234.86	233.69	0.52761	0.52505	0.16761	1.17	1.2343	1.2432		
			102		478.26	479.23			0.49880	0.51800	-0.77618					
			104		456.47	455.72			0.68762	0.67528	0.60783					
52	3	2	104	4	282.88	282.65	233.69	144.23	0.52505	0.56262	0.30757	89.46	0.3940	0.7343		
			102		479.87	479.21			0.51800	0.35187	0.89456					
			104		455.93	455.69			0.67528	0.74809	0.32429					
53	2	1	105	5	284.23	283.12	39.46	32.70	0.30757	0.00800	0.96719	6.76	1.0316	1.1433		
			102		480.65	480.58			0.89456	0.96225	0.06000					
			104		456.47	456.19			0.32429	0.27204	0.24688					
54	3	1	105	5	284.23	283.61	144.23	141.48	0.56262	0.54365	0.53514	2.74	1.1203	1.1521		
			102		480.65	479.81			0.35187	0.32217	0.72592					
			104		456.47	456.97			0.74809	0.77501	-0.43205					
55	2	1	104	2	282.88	283.13	32.70	11.00	0.00800	0.32917	-0.29946	21.70	0.4548	0.8595		
			103		482.94	482.14			0.96225	0.67281	0.93624					
			104		456.47	456.63			0.27204	0.66255	-0.18380					
56	3	2	105	11	284.23	284.06	141.48	85.51	0.54365	0.62310	0.21580	55.97	0.4054	0.7888		
			102		480.65	480.08			0.32217	0.15843	0.72495					
			104		458.12	457.61			0.77501	0.76593	0.65412					
57	3	1	105	10	285.58	284.75	85.51	72.84	0.62310	0.55429	0.88502	12.68	0.7073	0.9319		
			102		479.87	480.25			0.15843	0.22802	-0.41268					
			104		458.66	458.46			0.76593	0.80048	0.21549					
58	2	1	105	7	284.23	284.34	5.97	2.40	0.21580	0.42668	-0.09376	3.58	0.6919	1.1693		
			103		482.16	481.02			0.72495	0.24689	0.97962					
			104		458.66	458.45			0.65412	0.87005	0.17764					
59	3	2	105	4	285.58	285.52	72.84	64.82	0.55429	0.57935	0.05349	8.01	0.9096	1.0200		
			102		479.87	480.57			0.22802	0.34724	-0.68770					
			105		460.31	459.57			0.80048	0.73741	0.72403					
60	3	1	105	5	284.23	285.62	64.82	64.81	0.57935	0.58327	-0.77138	0.02	1.8087	1.8093		
			102		480.65	480.63			0.34724	0.34723	0.01006					
			105		460.85	459.70			0.73741	0.73432	0.63629					
61	3	2	105	11	284.23	286.35	64.81	64.81	0.58327	0.58331	-0.74014	0.00	2.8696	2.8696		
			102		480.65	481.06			0.34723	0.34724	-0.14474					
			105		462.50	460.62			0.73432	0.73428	0.65669					
62	3	1	106	5	286.93	286.17	64.81	53.07	0.58331	0.52043	0.80659	11.74	0.6536	0.9416		
			102		480.65	480.96			0.34724	0.43385	-0.32551					
			105		460.85	460.39			0.73428	0.73548	0.49342					
63	3	2	106	11	286.93	287.02	53.07	52.56	0.52043	0.52582	-0.06649	0.51	1.3560	1.3684		
			102		480.65	481.66			0.43385	0.46794	-0.74207					
			105		462.50	461.59			0.73548	0.71031	0.66701					
64	3	1	106	7	286.93	287.39	52.56	48.36	0.52582	0.58977	-0.43094	4.20	0.9409	1.0713		
			103		482.16	481.99			0.46794	0.47268	0.15719					

			105		463.04	462.09			0.71031	0.65479	0.88859			
65	3	2	106	8	288.28	287.68	48.36	31.79	0.58977	0.52631	0.63819	16.56	0.5618	0.9327
			103		482.94	482.23			0.47268	0.34218	0.76430			
			105		462.50	462.42			0.65479	0.77840	0.09255			

RESULTS OF CASCADE

9 VACANCIES

4 BERYLLIUM INTERSTITIALS

5 OXYGEN INTERSTITIALS

-0 SPUTTERS

PENETRATION OF PRIMARY
32.92 ANGSTROMS

OCCUPANCY OF LATTICE SITES AND INTERSTITIALS

AFTER COLLISION CASCADE

BOX	I I I I	I I I I	I I I I	I I I I
	123456 789XYZ *	123456 789XYZ *	123456 789XYZ *	123456 789XYZ *	123456 789XYZ *
99 99 101	B *	*	*	*	*
100 100 100	OV *	V *	*	*	*
101 100 101	B V *	O *	*	*	*
102 101 101	V *	VV *	*	*	*
103 101 101	B *	B *	*	*	*
104 101 102	O *	* B	*	*	*
104 102 103	V *	V O *	*	*	*
105 102 104	O V *	*	*	*	*
106 102 105	I *	*	*	*	*
0 0 0	*	*	*	*	*

VI. REFERENCES

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FLIGHT PROPULSION LABORATORY DEPARTMENT

GENERAL ELECTRIC