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MASTER

QUARTZ: A NUMERICAL SIMULATION OF AN ASYMMETRIC ELECTROSTATIC ACCELERATOR

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I. INTRODUCTION

A number of computer codes exist for the numerical modeling of axially symmetric, electrostatic accelerators [1-4]. However, for purposes of beam steering, it appears that it will be necessary to offset one or more electrodes, thus breaking the cylindrical symmetry of the device. Although an averaging scheme for construction of approximate potentials in such an asymmetric accelerator does exist [5], there is, to our knowledge, no computer code which directly obtains such solutions.

We have developed such a code, which we call QUARTZ. Important features of QUARTZ include the following:

1) use of a finite element code to obtain solutions of Poisson's equation in an asymmetric, three-dimensional volume,
2) inclusion of space charge neutralization by electrons,
3) inclusion of ion space charge through an iterative procedure.

The physics of the problem will be discussed in Section II, and the numerical techniques in Section III.

II. PHYSICS OF THE PROBLEM

A. Equations

The neutral injector problem reduces to simultaneous solution of two time independent partial differential equations. One of these is a modified form of Poisson's Equation:

$$\nabla^2\phi = -\frac{e}{\varepsilon_0} n_i(\vec{r},\phi) + \frac{e}{\varepsilon_0} n_{eo} e^{-\frac{e}{kT_e}(\phi_o-\phi)} \qquad (1)$$

where:

e is the charge of an electron

ε_0 is the permittivity of free space

k is Boltzmann's constant

T_e is the electron temperature

ϕ_0 is the potential at the center of the source plasma

n_{eo} is the electron number density at the center of the source plasma

$n_i(\vec{r},\phi)$ is the ion number density.

The other is the time-independent Vlasov Equation:

$$\vec{v}\cdot\nabla f + \frac{q}{m}(-\nabla\phi)\cdot\frac{\partial f}{\partial \vec{v}} = 0 \qquad (2)$$

where

q is the charge of an ion

m is the mass of an ion

$f = f(\vec{r},\vec{v})$ is the ion distribution function

The two are connected by the ion density n_i, which is the integral over velocity space of the ion distribution function f.

$$n_i(\vec{r}) = \int d^3v f_i(\vec{r},\vec{v}) \qquad (3)$$

Direct solution of the Vlasov Equation is, in general, extremely difficult, and so we will not attempt a direct solution. Instead we will solve only the modified form of Poisson's Equation, obtaining the unknown ion charge density n_i indirectly through an orbit tracing technique.

Thus we are not actually solving the Poisson-Vlasov system in the rigorous sense. We are solving a modified, nonlinear form of Poisson's Equation and obtaining part of the nonlinear term through a modeling technique.

The procedure used is almost identical to one used in a number of other attacks on the problem [1-4]. It is:

1) With zero space charge, solve Laplace's Equation in the volume of interest.

2) From the potential thus obtained, calculate electric fields, and use these to trace ion trajectories through the volume.

3) Use the trajectories to determine the amount and distribution of the space charge present in the volume.

4) The space charge obtained in 3), together with the electron contribution to the space charge, now becomes the inhomogeneous term for a new solution of Poisson's Equation.

5) Return to 2), and continue the procedure until the solution converges.

A flow chart of QUARTZ is shown in Figure 1.

B. Boundary Conditions

As shown in Figure 2, the beamlet under consideration is, in general, surrounded by six other beamlets. The plane which bisects the line connecting the center of our beamlet with the center of any of the other six beamlets is a surface of approximate reflection symmetry. The normal derivative of the potential must therefore be zero on each of these surfaces, and thus our problem volume is contained within an equilateral hexahedron on which the Neumann boundary condition

$$\frac{\partial \phi}{\partial n} = 0 \tag{4}$$

holds. We choose in the present model to approximate the hexahedron with a cylinder and impose the boundary condition

$$\frac{\partial \phi}{\partial r} = 0 \tag{5}$$

on the cylinder.

This condition does not hold on the electrodes themselves. Here the potentials themselves are known, and instead of the Neumann condition above we have the Dirichet condition:

$$\phi = \text{known value} \quad . \tag{6}$$

Particle trajectories begin on an equipotential surface. The potential of the surface is known, and is in general a few volts higher than the potential of the first electrode. This surface forms the left-hand boundary of our problem volume.

The right-hand boundary is also a surface of known, generally zero, potential.

We thus have specified either the potential or its normal derivative over the entire surface enclosing the problem volume. Together with specification of the ion and electron charge densities, this defines a well-posed boundary value problem for Poisson's Equation, and we are thus guaranteed the existence of a unique, stable solution of Poisson's Equation at each stage of the iteration procedure. We are not, however, guaranteed the convergence of the iteration procedure as a whole.

C. Equations of Motion

The Hamiltonian for a particle moving in a potential ϕ is:

$$H = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) + q\phi \tag{7}$$

where:

m is the mass of the particle,
q is the charge of the particle,
p_x, p_y, p_z are momenta in the x, y and z directions respectively.

The equations of motion, in Hamiltonian form are:

$$\begin{aligned} \frac{dx}{dt} &= \frac{p_x}{m} & \frac{dp_x}{dt} &= -q\frac{\partial\phi}{\partial x} \\ \frac{dy}{dt} &= \frac{p_y}{m} & \frac{dp_y}{dt} &= -q\frac{\partial\phi}{\partial y} \\ \frac{dz}{dt} &= \frac{p_z}{m} & \frac{dp_z}{dt} &= -q\frac{\partial\phi}{\partial z} \end{aligned} \qquad (8)$$

These six equations are solved either by making approximations to the force which allow analytic solution, or by use of the integrator ODE [6].

D. Initial Conditions for Ion Trajectories

The trajectories of the ions used to model the ion charge density may be started on an arbitrary emitting surface. Following Reference 1, we choose this surface to be the classical sheath edge, and call the sheath edge potential ϕ_s. Starting positions are distributed uniformly over this surface, corresponding to uniform source brightness.

The one dimensional sheath problem has been examined in detail by Self [7], who gives the following expression for the ion current density at the classical sheath edge:

$$j_+(n_s) = n_{eo} e I(n_s) \sqrt{\frac{2kT_e}{m_i}} \quad . \qquad (9)$$

where:

m_i is the ion mass,
T_e is the electron temperature
$n_s = e(\phi_o - \phi_s)/kT_e \approx .854$
$I(n_s) = 0.3444$

Values of the components of the initial momenta must be chosen consistent with this current. In the two dimensional treatment of Reference 1, it was assumed that the ion distribution at the sheath edge is a Maxwellian drifting in space with velocity v_D. In this case, we have the distribution function:

$$f_i(v,\theta) = n_{eo} e^{-n_s} \left(\frac{m_i}{2\pi k T_i}\right)^{3/2} \exp\left(\frac{-m_i}{2kT_i}\left[(v\cos\theta - v_D)^2 + v^2\sin^2\theta\right]\right) . \quad (10)$$

where T_i is the ion temperature of the source plasma. Jaeger has shown that this leads to an average longitudinal velocity equal to the drift velocity

$$\langle v_{long} \rangle = v_D, \quad (11)$$

while the average transverse velocity is

$$\langle v_r \rangle = \frac{\sqrt{\pi}}{2}\sqrt{\frac{2kT_i}{m_i}} \quad (12)$$

Further, we must choose as the drift velocity:

$$v_D = e^{n_s} I(n_s) \sqrt{\frac{2kT_e}{m_i}} \quad . \quad (13)$$

Thus the average longitudinal velocity of the emitted particles depends mainly on the electron temperature, while the average transverse velocity and the characteristic width of the velocity distribution depends on the ion temperature.

In the present version of QUARTZ, we have chosen to simplify the initial conditions somewhat. We assume that all trajectories leave the emitting surface at velocity v_D in a direction parallel to the longitudinal axis of the accelerator. This corresponds to an assumption of zero ion temperature, i.e., neglecting both the transverse velocity components and the width of the longitudinal velocity distribution.

E. Space Charge Calculation

From the trajectories computed by the integration of Hamilton's equations, we must obtain a space charge which models that of the trajectories.

If a trajectory carries a current I and spends a time Δt in a given volume, the effective charge in the volume due to that orbit is:

$$Q = I\Delta t \quad . \tag{14}$$

We can readily obtain I. The current density at the emitting surface is given by Eq. 9, so the total emitted current is just

$$I_{total} = j_+(A) \tag{15}$$

where A is the area of the emitting surface. Initial particle positions are distributed uniformly over the emitting surface, and we wish to model a surface of uniform brightness, so this current must be divided evenly among all orbits

$$I_{traj} = \frac{j_+(A)}{N} \quad . \tag{16}$$

The ion charge deposited by this trajectory in time interval Δt is then just

$$Q = \frac{j_+ A \Delta t}{N} \quad . \tag{17}$$

III. NUMERICAL METHODS

A. The Modified Poisson Equation

Between tracing groups of trajectories, we must solve the modified Poisson Equation for a specified ion space charge. The ion space charge has been obtained from the previous orbit tracing. In order to incorporate

various geometries easily, a finite element code, MODEL [8], was used to obtain the potentials throughout the finite element mesh, given the ion space charge, the boundary conditions, and the exponential approximation for the electron space charge. The differential form of the equation is converted to an integral form using the Galerkin technique [9]. A banded matrix is constructed using standard finite element techniques. The resulting matrix equation is factored for solution using a modified Gauss-Choleski algorithm. After factoring once for a given ion space charge, several minor iterations are performed to obtain self-consistent potentials. These iterations consist of back substituting the factored band matrix together with a mixture of the old potentials and a portion of the new potentials:

$$\phi^{new} = \omega\phi^{new} + (1-\omega)\phi^{old} \tag{18}$$

where ω is the relaxation coefficient.

B. The Finite Element Net

The finite element code used to solve the modified Poisson Equation requires the user to specify the element structure into which the problem volume is decomposed.

An element is a part of the problem volume in which a solution to a differential equation is sought. The element is bounded by a number of points, which are called nodes. It is possible to choose elements bounded by various numbers of nodes, and the optimal choice may vary from problem to problem. In the present work, we have chosen to use "eight-node bricks", quasirectangular solids with one node at each corner, but no nodes anywhere

else. A few of our elements are degenerate "eight-node bricks" - elements in which two of the line segments bounding the brick have shrunk to zero length. These elements are shaped like wedges rather than rectangular solids, but they may formally be handled like non-degenerate elements.

Data furnished to the finite element code must include:

1. mesh location data,
2. connectivity data,
3. boundary condition data.

The information in 1) is calculated by a mesh generator incorporated in QUARTZ. A geometric description of the problem is obtained from the input, and a screening routine determines whether the problem is of a type the generator is designed to handle. The three cartesian coordinates for each node are calculated by the generator, while other routines determine the connectivity of the nodes. Connectivity data is strictly topological and is independent of the actual coordinates of the nodes.

The finite element Poisson solver must be told

1) which nodes are constrained by a Dirichlet boundary condition,
2) which nodes are constrained by a Neumann boundary condition,
3) the value of the potential at each Dirichlet node,
4) the value of the normal derivative of the potential at each Neumann node.

Detailed information on setting parameters and running the code will be presented in a separate report.

Figure 3 displays a finite element decomposition of the problem volume.

C. Mesh Parameters

In the input the problem geometry is specified as a stack of non-concentric disks. Other entries allow the user to tailor the mesh to the problem by placing the largest number of nodes (and thus achieving the best resolution) where the potential gradients and charge density gradients

are largest. These gradients will, in general, be largest near the emitting surface at the left-hand end of the problem volume. This occurs for two reasons:

1) The electron space charge density is significant only near the emitting surface, dropping off exponentially with the potential as the potential decreases to the right.
2) Near the emitting surface the ion velocities are small, leading to large effective ion space charge densities.

The large electron and ion space charge densities will approximately but not exactly cancel, producing large gradients in both space charge density and potential.

The user can obtain good spatial resolution in any region by making appropriate choices in the input data. Variables can be set to control the number of angular sectors into which the upper and lower angular portions of the problem volume are divided. In general, potentials should show only weak angular dependence, except possibly near the emitting surface. Variables are also available to control the fineness of the mesh in the radial and longitudinal directions.

A comment should be made about the costs, in computer time, of mesh refinement in the various coordinates. A large fraction of the running time of the code is used to solve large, banded symmetric systems of linear equations generated by the Poisson solver. The solution time for such systems increases rapidly with the bandwidth. The bandwidth depends on the connectivity, since it is determined by the maximum difference in the numbers of the nodes bounding any one element. The nodal numbering scheme results in elements packing a given stage of the accelerator all having identification numbers larger than any element packing a stage to the left, and smaller than those packing a stage to the right. An important consequence

of this is that addition of extra longitudinal sections will not increase the bandwidth and thus will cause only a small increase in running time. Longitudinal mesh refinement is relatively cheap. This is not true of azimuthal mesh refinement. Increasing the number of azimuthal sectors will increase the difference in the identification numbers of the nodes forming many elements. This will increase the bandwidth of the equation systems to be solved. Thus azimuthal refinement is expensive in computer time.

D. Effective Space Charge Calculation

We make the approximation that the particle has undergone uniform acceleration in each of the three coordinates during the time interval Δt. This is equivalent to assuming that the particle experiences a constant electric field during the interval, the same approximation made in the Lawrence Berkeley [2] code. If the initial and final momenta in one of the coordinates are p_i and p_f, and the time step is Δt, the average acceleration in the coordinate is:

$$a = \frac{p_f - p_i}{m\Delta t} \quad . \tag{19}$$

The trajectory in this coordinate is then just a parabola:

$$s = s_i + \frac{p_i}{m} t + \frac{1}{2} at^2 \quad . \tag{20}$$

We deposit equal amounts of charge at M points along this paralola, the points being equally spaced in time. Recalling Eq. (17), the amount of charge deposited at each point is:

$$Q = \frac{j_+ A \, \Delta t}{NM} \quad . \tag{21}$$

We do this for each time step on each trajectory, until all orbits have left the problem volume. This produces a series of points, each with an associated charge. The charge locations are sorted to determine which element they are in, and charges in the same element are added to obtain the total positive charge for the element. This charge, divided by the element volume, is the positive charge density for the element.

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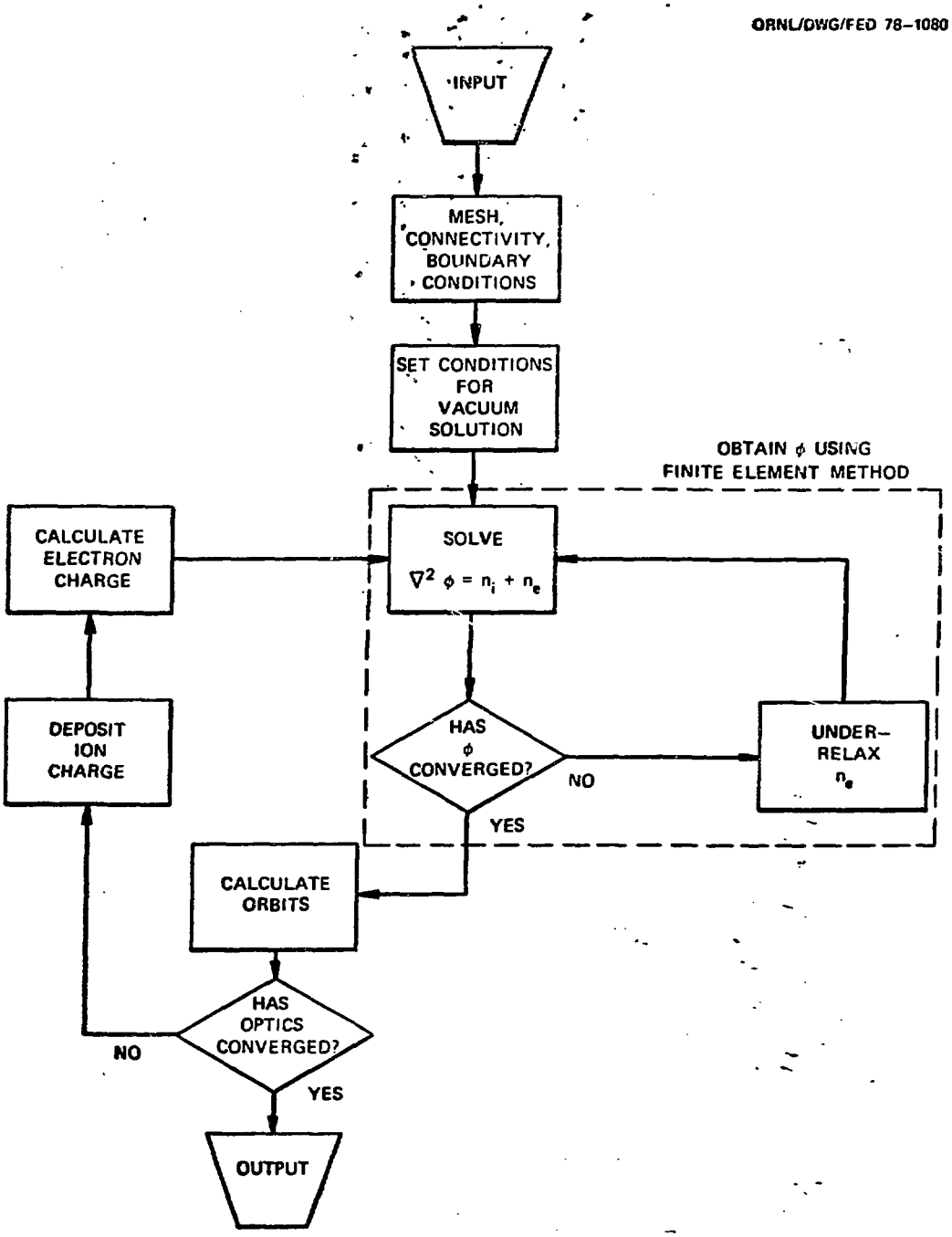
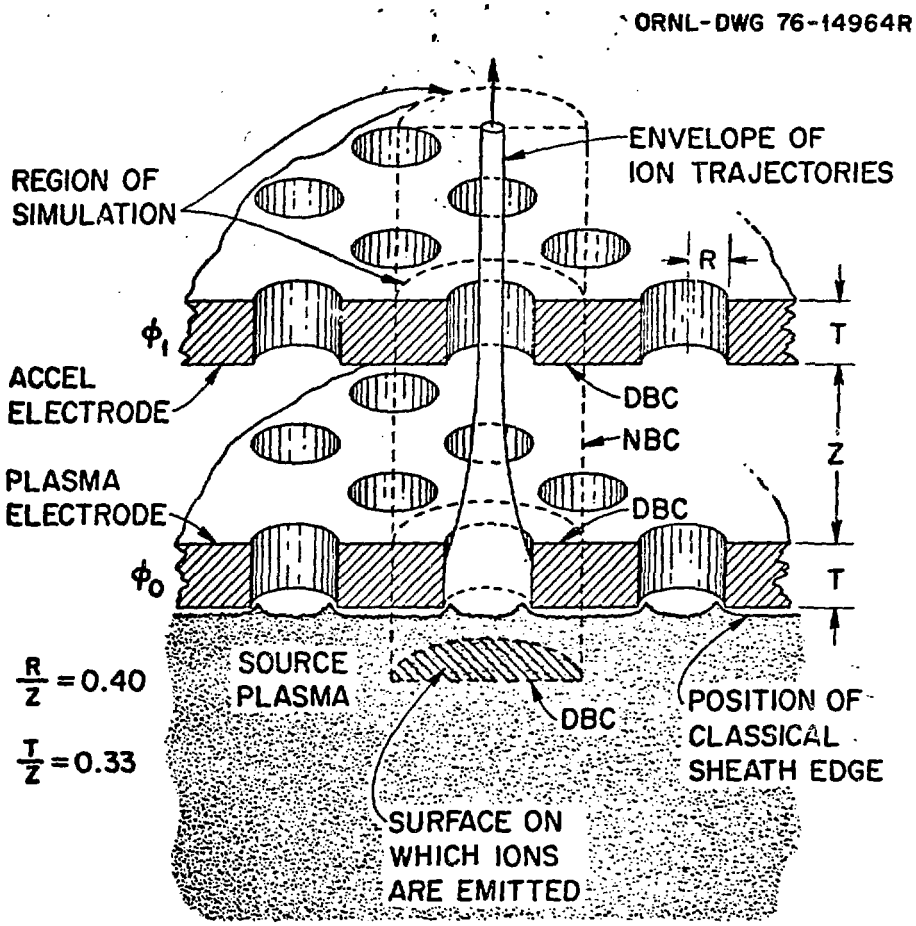
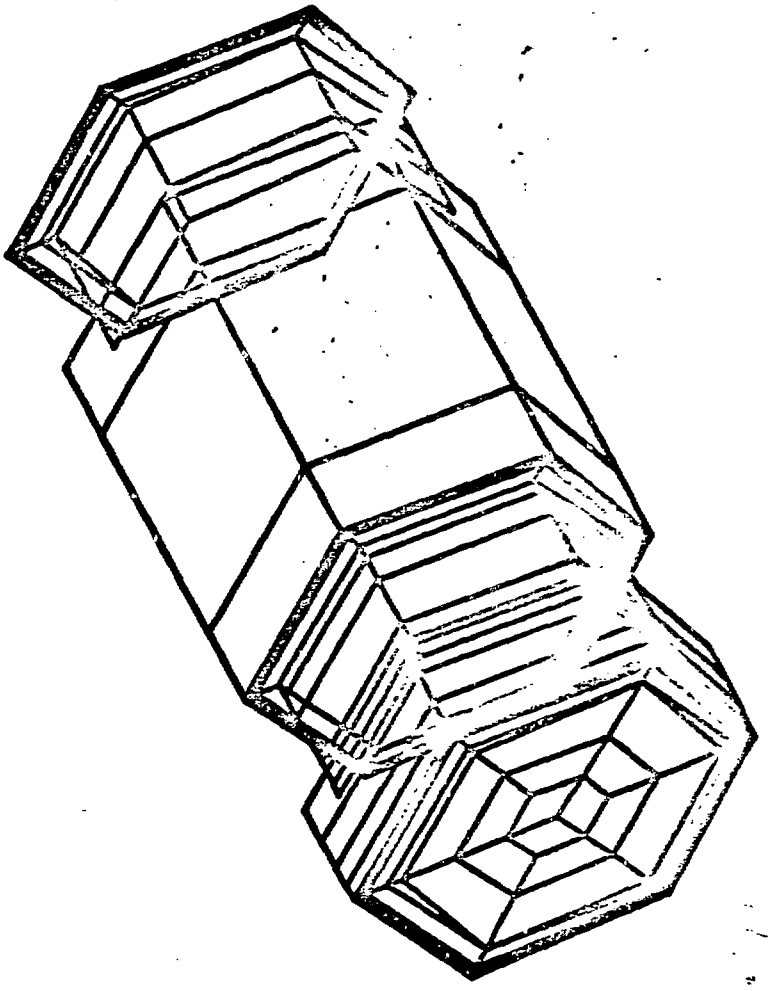

ORNL/DWG/FED 78-1080
INPUT
MESH, CONNECTIVITY, BOUNDARY CONDITIONS
SET CONDITIONS FOR VACUUM SOLUTION
OBTAIN φ USING FINITE ELEMENT METHOD
CALCULATE ELECTRON CHARGE
SOLVE
$\nabla^2 \phi = n_i + n_e$
DEPOSIT ION CHARGE
HAS φ CONVERGED?
NO
UNDER-RELAX n_e
YES
CALCULATE ORBITS
HAS OPTICS CONVERGED?
NO
YES
OUTPUT

Figure 1



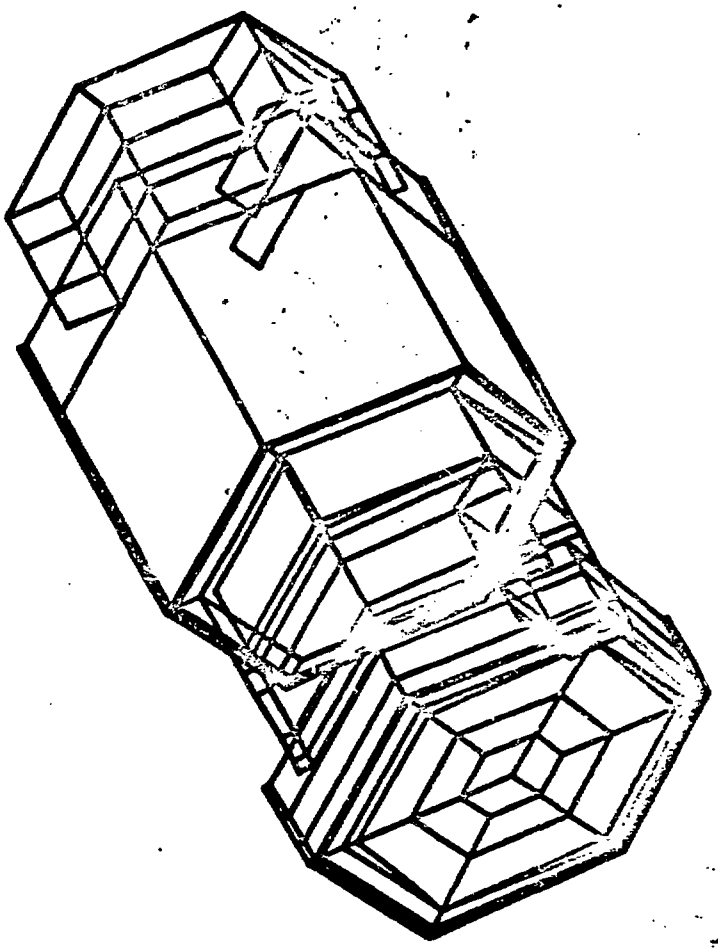
NBC - NEUMANN BOUNDARY CONDITION
DBC - DIRICHLET BOUNDARY CONDITION

Figure 2



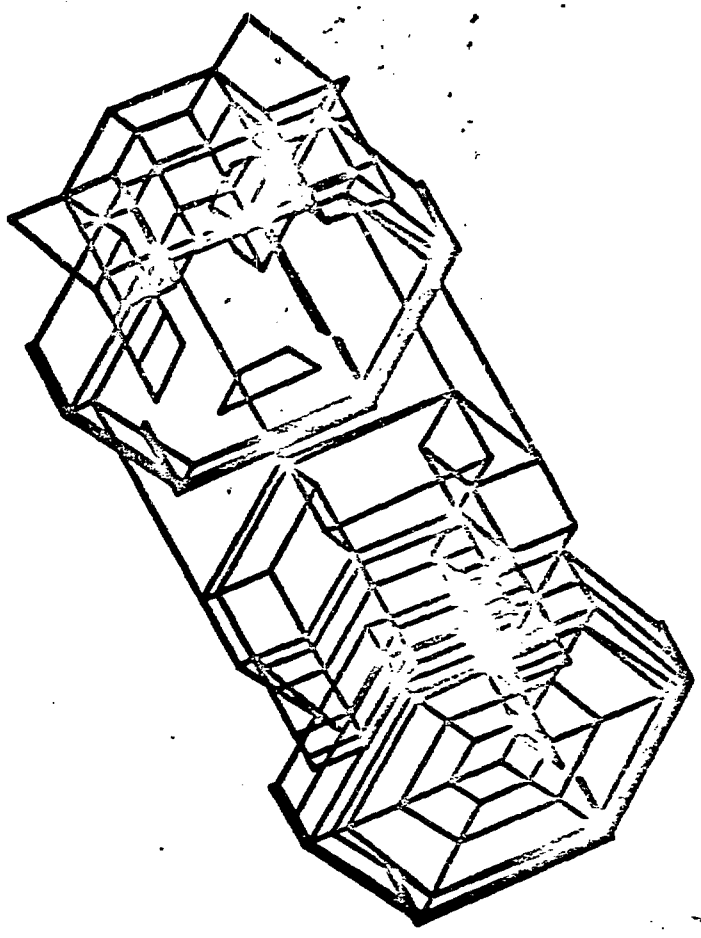
LAYER 1

Figure 3a



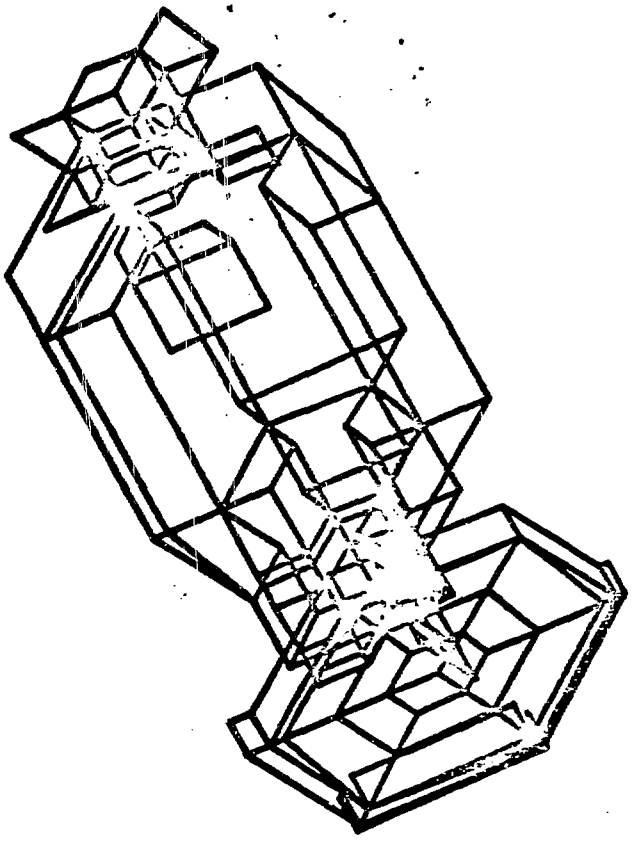
LAYER 2

Figure 3b



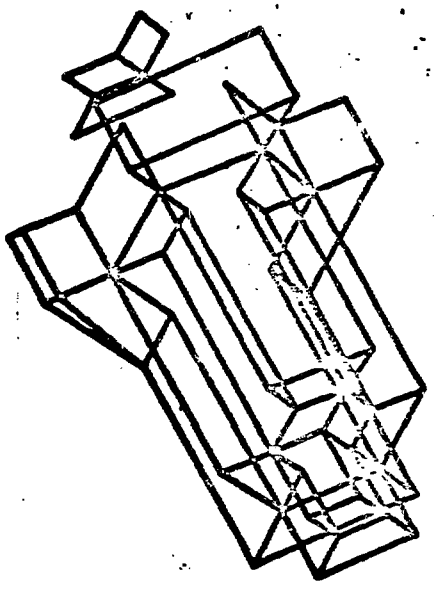
LAYER 3

Figure 3c



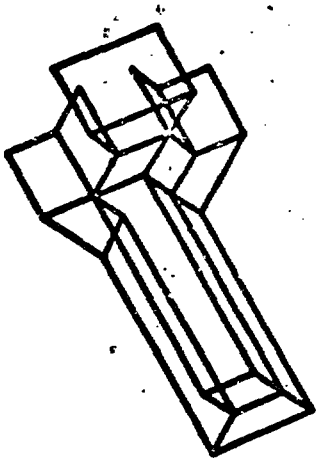
LAYER 4

Figure 3d



LAYER 5

Figure 3e



LAYER 6

Figure 3f

LAYER 7

Figure 3g

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