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COMPUTER PROGRAMS FOR THE TWO BODY
APPROXIMATION TO THE RADIATION
DAMAGE PROBLEM

JOHN P. BIRD
and
RONALD L. KRONZ

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COMPUTER PROGRAMS FOR THE TWO BODY
APPROXIMATION TO THE RADIATION DAMAGE PROBLEM

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and

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COMPUTER PROGRAMS FOR THE TWO BODY
APPROXIMATION TO THE RADIATION DAMAGE PROBLEM

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Submitted in partial fulfillment of
the requirements for the degree of

MASTER OF SCIENCE
IN
PHYSICS

United States Naval Postgraduate School
Monterey, California

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COMPUTER PROGRAMS FOR THE TWO BODY
APPROXIMATION TO THE RADIATION DAMAGE PROBLEM

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John P. Bird

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This work is accepted as fulfilling
the thesis requirements for the degree of

MASTER OF SCIENCE

IN

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from the

United States Naval Postgraduate School

ABSTRACT

A binary collision simulation of the radiation damage problem is proposed. Energy thresholds and parameter adjustment are discussed. Preliminary results show strong focusing in the (110) direction and weaker focusing in the (100) direction.

Although not complete, the model is expected, with suggested modifications, to adequately represent the radiation damage problem.

The authors wish to express their appreciation for the assistance and encouragement given them by Associate Professor Don E. Harrison, Jr. of the U. S. Naval Postgraduate School in this investigation. The authors also are pleased to acknowledge the assistance of Lt. Herbert L. Hoppe, USN, of the U. S. Naval Postgraduate School who was instrumental in the development of the binary collision interaction subroutine.

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1. Introduction

The interaction of energetic particles with matter may be divided into two energetic regions of interest:

- 1) High energy events in which interactions are primarily inelastic electronic processes of excitation and ionization, and
- 2) Low energy events in which the interactions are essentially elastic interactions between whole atoms.

There is an intermediate energy range in which both processes are important, but until the two limiting cases are better understood, attempts to understand the intermediate range seem futile.^{1*} The threshold energy for which electronic excitation and ionization processes become important depends upon the mass of the energetic particle. An approximate formula for this threshold energy is $E = A \text{ kev.}$, where A is the atomic mass of the energetic particle. The threshold for electronic processes seems to be relatively insensitive to the atomic mass of the target material.² For metals this threshold is of the order of 10-100 kev. The high energy processes of electronic excitation and ionization have received considerable attention and are reasonably well understood.³⁻⁶ We will confine our attention to the energy region below this threshold for inelastic electronic processes.

Many physical properties of a material are changed when the material is irradiated.⁷ The Young's modulus and the electrical

* All footnotes refer to the bibliography.

resistivity are among those properties of materials which show most significant changes. For metals and semiconductors, the residual electrical resistivity is most sensitive to radiation.

Semiconductors, for example, may show changes in electrical resistivity of up to four orders of magnitude,⁷ but there is no known simple relation between the magnitude of the change in electrical resistivity and the amount of radiative energy absorbed by a semiconductor. Radiation changes some semiconductors from n-type to the p-type.

The radiation damage problem involves chemical bonding between the atoms of the target material as well as elastic collisions between atoms. For low energy collisions, chemical bonding forces vary widely for different atomic species, but are of the same order of magnitude as the elastic repulsive forces. Therefore, to reduce the complexity of the problem, we have limited our investigation to simple crystals of face centered cubic metals, with special emphasis on copper.

Davies, et al. have developed a chemical technique for removing thin layers (≥ 37 A) from aluminum foils.⁸ The thickness of the layers is easily controlled. The technique has been widely used to study the range of radioactive ions in aluminum.^{9,10} Ranges have been measured for Cs¹³⁷, Rb⁸⁶, Na²⁴, and K⁴². For example, the mean range of 10.5 kev. Na²⁴ ions in aluminum was found to be about 250 Angstroms.

When a metal is irradiated with heavy energetic ions (≥ 50 kev.) a significant number of atoms are ejected from the target through the surface

which is bombarded by the incident ion beam. This phenomenon is known as sputtering. Under suitable conditions as many as 40 atoms or ions may be sputtered for each incident particle.¹¹ Examination of the angular distribution of sputtered particles reveals definite preferential ejection in directions which correspond to (110), (100), and (111) lattice directions.¹²⁻¹⁶

2. Lattice Effects

Whether a lattice atom leaves its original site or not after a collision depends upon the energy absorbed by the atom and its final direction of motion with respect to the lattice. If an energetic lattice atom does not leave its site, it will transfer energy to its neighbors through elastic collisions until thermal equilibrium is reached. Because of crystalline structure, the dissipation of energy is expected to be anisotropic. The only exception to the eventual thermalization of the excess energy of a bound lattice atom is the case in which sufficient energy reaches a surface of the material to knock one or more atoms away from the surface.

If a lattice atom is given sufficient energy to leave its site permanently, and no other atom replaces the energetic atom, a vacant lattice site is created. The surrounding lattice atoms relax slightly toward the vacant site, but the lattice structure remains essentially the same as that of a perfect lattice.¹⁷ The energetic atom travels through the lattice giving up energy through elastic collisions with the atoms near its path until it no longer has sufficient energy to force its way between the atoms of the crystal. If there are no vacant lattice sites near the position at which an energetic atom is brought to rest, it will be forced to occupy some position other than a regular lattice site.

Three possible equilibrium positions have been suggested for these interstitial atoms in a face centered cubic crystal: the crowdion, the split interstitial pair, and the center of a unit cell.¹⁷ The crowdion

consists of an extra atom in a (110) line of atoms. In the split interstitial pair configuration, the interstitial shares a regular lattice site with another lattice atom so that each is symmetrically displaced from the equilibrium position in a (100) direction. An atom in the center of a unit cell may also be described as a crowdion in a (100) direction. The lattice atoms surrounding an interstitial are displaced from their regular lattice sites to accommodate the extra atom. More will be said about the interstitial configuration later.

An energetic atom (knock-on) may transfer essentially all of its energy to a single lattice atom in a head-on collision.¹⁸ In this case, the lattice atom becomes the knock-on, leaving a site for the former knock-on to occupy. The new knock-on may, in turn, transfer essentially all of its energy to another atom. Thus, a chain of replacements may transport an interstitial to a position which is several times the distance between nearest neighbors from the corresponding vacancy. Replacement chains may be cyclic so that the last replacement in the chain fills the initial vacancy, leaving no vacancies or interstitials.¹⁷ The configuration consisting of a vacancy and a nearby interstitial, known as a Frenkel pair, may be stable or unstable. The stability of a Frenkel pair depends upon both the distance of separation and the orientation (with respect to the lattice) of the interstitial and the vacancy.

Silsbee has shown¹⁹ that an isolated line of hard spheres may focus and transfer energy along the line. The condition for focusing is that $s/d < \cos \beta$, where s is the distance between adjacent spheres,

d is the diameter of the spheres, and θ is the angle between the velocity of the first atom in the line and the line. The hard core approximation (diameter of spheres equal to distance of closest approach for a head-on collision) is useful in this work. For reasonable repulsive potentials such as the Coulomb, Bohr, Born-Mayer, etc., this modified model predicts a focusing effect below a threshold energy, and a de-focusing effect above this threshold energy.¹⁷ When the Gibson potential #2 simulates copper, this model predicts focusing in the (110) directions below about 60 ev., with sharp focusing below about 15 ev. The presence of adjacent lines of atoms will enhance the focusing effect found in an isolated line of atoms. Although the hard sphere models used to demonstrate the phenomenon of energy focusing contain rather drastic assumptions, the same sort of effect is expected from models based on more realistic potentials.

A channeling effect has also been reported.²⁰ This is the tendency for an energetic atom traveling in a (110) or (100) direction to be focused along a (110) or (100) line that is centered between surrounding (110) or (100) lines of lattice atoms. The energetic atom may travel a large distance along a channel compared to the distance it would travel in some other direction. The rate of energy loss along the channel is highly dependent on the potential function which governs the interaction, the energy of the atom, and its deviation from the line of focusing. From geometrical considerations, one would expect (100) channels to dissipate more energy per unit length than would be dissipated by (110) channels.

Channels, energy chains, and the displacement chains, then, may produce vacancies which are separated by large distances from their corresponding interstitials and sputtered atoms. Thus, chains and channels are competing mechanisms which produce the same effects. Energy and displacement chains should not be significantly affected by the presence of vacancies. Vacancies in the lines of atoms surrounding a channel should tend to divert channeled energetic atoms into the corresponding chains. Interstitial atoms should tend to disrupt channels and chains.

It appears that the chain and channel mechanisms are the dominant factors in the radiation damage event. The conditions for stability and the lengths of the chain/channels will then largely determine the final lattice configuration.

3. Theoretical Work by Others

Gibson, et al.¹⁷ have studied radiation damage events by integration of the classical equations of motion of the atoms in a small crystallite (< 1000 atoms). A central repulsive potential of the Born-Mayer type, $A \exp(-r/b)$, was assumed for the interactions between atoms. In order to contain the events it was necessary to restrict the energy to < 400 ev. Calculations were made on a high speed digital computer.

The computer program developed by Gibson, et al.¹⁷ keeps a record of position co-ordinates and velocity components for each atom in the crystallite. The orbits of the atoms are arbitrarily divided into segments with respect to time, i.e. time steps. In order to calculate the trajectories of the atoms for a particular time step, the atoms are considered sequentially. The resultant force on an atom under consideration is calculated from the position of the atom and the positions of the surrounding atoms. The atom is then moved for one time step under the influence of this resultant force. When the calculations are completed for all atoms for a given time step, calculations for the next time step are begun.

If the repulsive force between adjacent atoms were the only force simulated, the crystallite would expand without limit. Therefore, it is necessary that an attractive force act on the surface atoms of the crystallite. If all collisions were elastic collisions, and if the original energy (for a 100 ev. run) were completely contained in the lattice, the mean

energy of the atoms would be about 0.1 ev. after thermalization.

This corresponds to about 900° C. as the final temperature of a system which started at 0° C. Therefore, a viscous damping force was applied to surface atoms to dissipate energy.

This model is useful in studying low and moderate energy (<400 ev.) effects in radiation damage events. The effects studied were stability of lattice defects, anisotropy of energy transfer (energy chains), and displacement chains. Interatomic potential and surface effects were also studied.

In the Gibson model, energy chains play a dominant role in the dissipation of energy from the initial knock-on. Frenkel pairs are shown to be stable for distances of separation greater than 2 1/2-4 times the nearest neighbor distance, depending upon the orientation of the pair with respect to the lattice. Interstitials were studied extensively and found to be stable only in the split interstitial configuration.

Oen, et al.²¹ have investigated the stopping of energetic atoms (1-100 kev.) by solids. The model is based on binary elastic collisions between a primary knock-on and successive target atoms which are initially at rest. Lattice effects are neglected; the target atoms are initially randomly distributed throughout the target material.

The ultimate goal of the work by Oen, et al. is to discover the appropriate interatomic potential. The immediate aim is to calculate histories of many primaries which may be considered to simulate a

beam of incident atoms or ions .

Trajectories and histories are calculated only for the primary knock-ons , i.e. any effect produced by secondary knock-ons is neglected. The history of each primary consists of:

- 1) R, the distance from the initial position to the final position of the primary ,
- 2) X, the component of R parallel to the initial direction of motion of the primary ,
- 3) P, the component of R in a plane perpendicular to the initial direction of motion of the primary , and
- 4) L, the length of the path traversed by the primary .

Each run consists of the calculation of histories for enough primaries , usually 1000 , to insure that statistical fluctuations in the mean values of R, X, P, and L were acceptable ($< 3\%$).

The potential used was an exponentially screened Coulomb, or

Bohr potential:
$$V(r) = \frac{E_B}{2} \frac{\exp(-r/a_b)}{r/a_b}$$

where $E_B = 2Z_1 Z_2 e^2/a_b$ and $a_b = k a_H / (Z_1^{2/3} + Z_2^{2/3})^{3/2}$

where a_H = first Bohr radius (0.529 A). The parameter k may be adjusted to achieve agreement with experimental results. The hard sphere approximation to the Bohr potential was also used in some cases for comparison.

Results for the cases of 10.5 and 60 kev. Na^{24} ions incident upon aluminum targets were compared with the experimental results of Davies & Sims.⁸ No serious discrepancy is found in the mean penetration, \bar{X} .

However, the experimental distribution of penetration is more "skewed" toward lower penetration than the distribution of penetration calculated by Oen, et al.

4. The Problem

The binary collision model has been the basis of all analytical studies of radiation damage and sputtering. Many machine calculations have been made in recent years using an N - body collision model. However, no serious attempt has been made to determine whether or not a two-body approximation would yield satisfactory results.

Our problem, then, was to build a model based on the binary collision whose logic would be sophisticated enough to adequately represent the radiation damage problem. The nature of the results obtained would then definitely establish the degree of confidence to be placed in any binary collision approximation models.

5. The Binary Collision

With minor modifications, any repulsive potential may be used in the two body interaction. An eroded form of the potential is used, i.e. the potential has a definite radius of effect. We have taken this radius of effect (or sphere of influence) as an input parameter, SPHI. There is, then, no interaction between atoms whose separation is greater than SPHI.

All applications of the program to date have used an eroded Born-Mayer potential, $V = A \exp(B(1-r/SPHI))$ for $r \leq SPHI$. The constants A & B were taken from Gibson et al. for three different Born-Mayer potentials, termed simply Potentials, 1, 2, and 3. The constants for these three potentials are:

POTENTIAL	A (ev.)	B
1	.0392	16.97
2	.0510	13.00
3	.1004	10.34

The interaction starts with the two atoms at SPHI distance of separation with all the energy as kinetic energy. All co-ordinates and velocity components are transformed to the center of mass system, where the equations of motion are:

$$1) \quad dt = (2/m' (E-V-L^2/2m'r^2))^{-1/2} dr$$

$$2) \quad d\theta = (L/m'r^2) dt$$

where t = time
 m' = reduced mass
 E = kinetic energy
 V = potential energy
 L = total angular momentum
 r = distance of separation
 θ = angle of deviation
 s = impact parameter

The equations are integrated from $r = \text{SPHI}$ to $r = \text{CPA}$, the distance of closest approach. Since the interaction is symmetrical in the center of mass system, the definite integrals of the above equations are one-half the time of interaction and one-half the total angular deviation, respectively.

CPA is found by an iteration of the formula:²²

$$(\text{CPA})^2 (1 - V(\text{CPA})/E_r) - s^2 = 0$$

The first approximation to CPA is taken as SPHI. A four point Gauss-Legendre quadrature is employed to evaluate the integrals.²³

6. Development of the Model

When the possibility of a feasible two body approximation to the radiation damage problem is considered, two major problems are immediately encountered.

The atoms would, of necessity, be considered in some sort of ordered sequence, but all calculations for a single atom could not be carried through before the other atoms are considered since this would obviously leave out of the calculations the effect of collisions suffered by other atoms. This first major problem led to the time step approach, and eventually to the use of an absolute time of an atom's last collision.

The second major problem is to develop a mechanism which will handle simultaneous collisions within a two-body approximation.

After the program was developed, we discovered that the lattice would not hold together which necessitated a further modification. This difficulty is only partially resolved.

The first question considered in the development of the model was to mathematically create a face centered cubic lattice in table form, together with a method which tags each atom so that its subsequent movements and initial position could be found. Figure 2, APPENDIX II, shows the ordered arrangement found in a (100) plane of a fcc lattice. The distance between two atoms along the (100) direction is taken as two units. It will be noted that if the total X dimension, IX , is odd, then there are an equal number of atoms in the line $y = 0$ and the line $y = 1$. By specifying IX odd, the number of atoms in a line $y = \text{constant}$

is known to be $(IX + 1)/2$. This value, $NLINE$, can then be multiplied by the total Y dimension plus one $(IY+1)$, and the number of atoms in the whole plane, $NPLANE$, is obtained. It will be noted from Figure 3 that the next plane, one Z unit removed, is akin to a photographic negative of the plane under consideration. However, the ideas of $NLINE$ and $NPLANE$ are still valid. The total number of atoms in the lattice can then be found by multiplying $NPLANE$ by the Z dimension plus one $(IZ+1)$. If the atoms are numbered sequentially as shown in APPENDIX II, the initial co-ordinates of their sites can also be found by the method shown in APPENDIX II and APPENDICES IV & V (BOX 31).

The process outlined above will create and number a 1500 atom lattice in approximately one second. An advantage of this method is that a rectangular lattice of any size or shape desired can be created by specifying IX , IY , and IZ . The only restriction is that IX must be odd.

The atoms are now considered sequentially, for a period of one Time Step Length (TSL), and all collisions that will take place before the end of the time step are allowed to happen. All atoms are then moved to points in space and time corresponding to the end of the time step, and the process is repeated for the next time step.

The length of a time step was originally calculated so that the most energetic atom in the lattice could move one lattice unit (1.807 Angstroms for copper) in one time step. This has been modified so that it is now able to move any desired fraction, $TFAC$, of one lattice

unit. TFAC is, naturally, one of the input parameters of the problem.

Since the energy of the most energetic particle, ENERGY, in the lattice decreases during the course of the run, the TSL should be recalculated periodically for greater efficiency. Provisions were made to recalculate the Time Step Length every JPB (an input parameter) time steps. The TSL is also recalculated every time another particle is shot into the lattice, since it is assumed that this particle will be the most energetic one present, and it was not thought feasible to wait for the next regular recalculation. A table of the first 30 Time Step Lengths, and the time step of recalculation, is kept for reference.

As now constituted, there are one external and two internal methods used to determine the number of time steps which complete a run. The external method is the only one available to the operator once a computational run has commenced.

First, a variable limit is set on the maximum number of time steps (MNTS, an input parameter) that may be taken. The calculation must cease when this number of time steps has been completed, and the results are then obtained.

Second, the program, at the beginning of each time step, decides whether or not it should continue for another time step. The decision to continue is made if the energy of the most energetic particle (called ENERGY) in the lattice (excluding all those that have left the lattice) is greater than a certain threshold energy, THERMAL (an input parameter explained below). If ENERGY is less than THERMAL, the run is

considered completed and the informational output is given.

Third, the operators may decide to shut down operation before either of the two internal limits have been reached. This may be done at any time, simply by throwing a switch, and the computation will cease at the beginning of the next time step.

The external mode of problem completion should not be the normal operating condition, nor should the number of time steps be allowed to approach MNTS under most conditions, since either method still leaves atoms in the lattice with more energy than the quantity THERMAL. Usually the calculation should cease of its own accord, with the second method given above as the basis for the internal decision. Other factors, such as running time, mechanical failures, etc., may necessitate the use of the external method, but these are to be avoided if possible.

A method of program regeneration was also devised so that the run could be discontinued at the start of any time step and then restarted at that point at some later time. This has definite value where continuous periods of available machine time are not long, or when mechanical or electrical failures destroy the calculations. The information needed for regeneration can be obtained at the beginning of any time step and the calculation continued (or stopped if desired).

In this manner, if the calculation has been running for three hours before a failure of some kind occurs, the only time that need be repeated on the machine is the time elapsed since the last regeneration

information was put on magnetic tape. It should be noted that the regeneration need not be undertaken at once, but may be delayed until convenient. This regeneration process has great practical importance to the user of the program, but is of no theoretical value.

Many atoms are given only a cursory examination during a time step, while the more energetic atoms are subjected to a highly detailed treatment. The use of two energy thresholds in the model simplifies this choice for a particular atom.

ETHRESH, the upper energy threshold, is the energy required for an atom to move from its site to a site near it, i.e. the displacement energy. Calculations by others¹⁷ have shown this displacement threshold to exist, and also that it is in the neighborhood of 20 electron volts. They have also shown¹⁷ that this displacement threshold depends upon direction, and is lower in the (100) and (110) directions than in other directions in the lattice. This directional dependence of the displacement threshold has not been built into the present model, but it should be considered in any future development of the model.

THERMAL, the lower energy threshold, is an arbitrary dividing line imposed upon the model, below which atoms are quite arbitrarily placed on sites or formed into interstitial pairs with other atoms and not allowed to move. Atoms above THERMAL are allowed to participate normally in collisions.

There are, then, three distinct energy classes among the atoms in the lattice:

- 1) Those with energy above ETHRESH,
- 2) Those with energy between ETHRESH and THERMAL, and
- 3) Those with energy below THERMAL.

The three classes will be discussed separately.

The atoms above ETHRESH do not occupy a site in the lattice, collide with other atoms as necessary, and obtain information about their subsequent motion only from the interaction subroutine.

The atoms between ETHRESH and THERMAL are forced to occupy specific lattice sites, but are allowed to vibrate around these sites. They cannot move to a new site because their energy is less than the displacement energy. These atoms are allowed to move undisturbed until they have a collision, and then after the collision has been completed, if they lose a specific percentage, TURN (an input parameter), of their original energy their velocity vectors are changed to point back toward the site occupied by the atom.

We found prior to the use of this turn-around method that the lattice had no inherent cohesiveness. This method holds the lattice together.

To speed up computation time, atoms with energy below THERMAL are forced to occupy a fixed site, or to share an interstitial site with a partner, and are not allowed to move. This is a reasonable and valuable approximation for atoms of low energy, since they will not have an

appreciable effect on the results of the computation. The energy and associated velocity components of these thermalized atoms are kept intact for use in possible future collisions.

After the decision is made to continue for another time step, and the Time Step Length has been recalculated, the atoms are considered sequentially. The information associated with the atom under consideration (primary atom) which is stored in the LB array is first inspected. If the atom has:

- 1) An energy equal to or less than THERMAL, or has
- 2) Been through the current time step, or has
- 3) Left the lattice,

we move on to consideration of the next atom.

We will account for all collisions if we consider only those atoms with energy greater than THERMAL, since atoms with energy less than THERMAL are not allowed to move unless hit. Atoms that have already been through the time step have completed all interactions which occur during the time step and should not become involved again until the next time step. Atoms that have left the lattice will not be considered for the remainder of the problem.

A primary atom with energy above THERMAL is finally selected, or the computation shuts down. A list of all other atoms it is possible for this atom to hit in this time step is required. To shorten the computation, a mathematical box is constructed around the atom in question (hereafter referred to as atom M) and a list (the NUM list) is made of

all atoms whose positions (centers) are inside the box. If the box is made large enough, it will be impossible for atom M to hit any atoms outside the box, so we need consider only those on the NUM list. At present, the box is given sides of 3.02 units, or ± 1.51 units. Initially, the sides were ± 1.01 , but this has been found to be too small, and obvious collisions were missed. Atoms that have been through the time step are not included on this list, since their co-ordinates are relative to the end of the time step rather than the start of the time step. Atom M is placed first on the list for programming facility and easy reference.

The impact parameter between every other atom on the NUM list and atom M is then calculated, these distances comprise the DSTANCE list. The time at which each atom reaches this distance of closest approach, and the time at which the atom and atom M are SPHI (sphere of influence of an atom) distance apart are also calculated. These times are placed on the TMIN and T lists, respectively.

During the course of the calculation of the DSTANCE, TMIN, and T lists, several tests are performed on these quantities. If the DSTANCE for an atom is larger than SPHI, no collision will occur. If the relative velocity is less than 10^{-6} , then the atoms are moving very slowly relative to one another, and the collision is ignored. Several tests are then performed on each T. If the time T is less than the start of the preceding time step, it would have been considered in this previous time step, and is therefore treated as a spurious collision. If the time T is greater than the end of the current time step, it will be re-examined in

the next time step. The times of the last collision of atom M and the other atom are then checked, and if the time T, on an absolute scale, is less than either of these, the collision is spurious since it would be starting before one that had already taken place. The last test performed is whether the time T is within .00001 (TSL) of the end of the time step. If so, we feel that it would be better to consider this collision in the next time step, since to consider it now would mean that the end of the collision was far into the next time step, which is unsatisfactory from a practical viewpoint.

If, after this series of eliminations, there are no atoms left, then atom M is moved to the end of the time step, and the next atom in sequence becomes atom M.

If atoms remain on the list we select the ones that atom M will hit. Two alternative methods of selection were considered by the authors:

- 1) Select the one, or ones, that are closest (i.e. a space-wise selection), or
- 2) Select those that will collide with atom M first (i.e. a time-wise selection).

Only the second method has been used.

The space-wise selection would surely include all the hardest collisions, and would probably be easier from a programming viewpoint. However, a time-wise selection insures that atom M will hit first what it really should hit first. Atom M may thereby miss a hard collision with another atom because of another previous soft one, but we

currently feel that this is a truer picture of what actually happens in the lattice during the radiation damage process. We feel that both methods should be tried in future development of the model. A study as to the relative feasibility of both methods would enhance the usefulness of the model.

Atoms are selected that have the smallest times, T . Since we assume that two atoms have no interaction if they are separated by a distance greater than $SPHI$, the time T is the actual time of collision. We feel that some leeway should be available here, therefore all atoms whose times T are within a certain amount (CUTOFF) of a time step from the minimum times are also selected. These atoms are placed on the KHIT list, with atom M first on the list. Since CUTOFF is an input parameter, adjustment to a satisfactory value may be accomplished easily. Use of the CUTOFF parameter also eliminates some of the objections to the time-wise selection process.

The initial velocity components and energies of all atoms on the KHIT list are then stored in the SAVE array because they will be needed for the velocity scaling processes.

It must be emphasized that atom M hits all those on the KHIT list almost simultaneously. This necessitates some sort of energy and velocity scaling process, or a general solution to the N body problem.

We feel that if the two body approximation is to have any validity atom M must enter into each of the two body collisions with its initial energy, but the program must scale the results in some fashion. Assume,

for example, that M initially has an energy of 100 ev. and hits two atoms simultaneously with identical impact parameters. It is more feasible to assume that M hits each one with an energy of 100 ev. than to assume that M hits one with 100 ev. and hits the other with whatever energy is left, say 37 ev.

Naturally, with M hitting each atom separately with 100 ev. the struck atoms will receive too much energy, we must therefore scale the results.

In the actual collision process of the model, then, atom M and the next atom on the KHIT list are moved to their calculated positions at the time T for the atom being hit. The collision is then calculated and the struck atom is given its new position co-ordinates, velocity components, and energy. Atom M and the next atom on the KHIT list are then moved to the positions corresponding to their actual time of collision, T, and so forth. This is repeated until atom M has "struck" all the atoms on the KHIT list.

To conserve both energy and momentum in any scaling process would constitute a general solution to the N body problem. We, therefore, elected to conserve energy rather than momentum, feeling that this would give us a more realistic insight into the radiation damage problem.

There are four general scaling cases that must now be considered:

- 1) Atom M "lost" more energy than it started with,
- 2) Atom M "lost" exactly all the energy it started with,

- 3) Atom M started with an energy above ETHRESH and did not "lose" all of its energy, and
- 4) Atom M started with an energy below ETHRESH, but above THERMAL, and did not lose all of its energy.

These cases will be discussed in order.

CASE I

Atom M is allowed to lose all its initial energy, and its velocity components and energy are set equal to zero. The energies and velocities of the struck atoms are then scaled to conserve energy. The energy scaling factor used in this case is simply the total energy (of those on the KHIT list) before the collisions divided by the total energy after the collisions. The velocity scaling factor is the square root of the energy scaling factor. The energies and velocities of all atoms on the KHIT list, except atom M, are scaled by these two scaling factors.

Both energy and the absolute velocity directions are conserved by this process.

CASE II

Atom M is allowed to lose all of its initial energy, and its velocity components and energy are set equal to zero. Here, however, energy scaling is not necessary since energy has already been conserved.

CASE III

Here it is not necessary to scale the energies of the struck atoms, since atom M did not lose all of its initial energy, so the struck atoms retain the energies and velocities they received in the two body collision

process. The energy of M is found by subtracting the energy gained by the struck atoms from M's initial energy. M's velocity components must now be found.

The sums of the individual velocity components calculated for M, but not given to M, are taken. Call these sums S_1 , S_2 , and S_3 for the X, Y, and Z directions. Let R be $(S_1^2 + S_2^2 + S_3^2)^{1/2}$. The magnitude of M's final velocity, V, is known since the energy is known. The X velocity is then taken as $(V/R)(S_1)$, and similarly the Y and Z velocities are $(V/R)(S_2)$ and $(V/R)(S_3)$ respectively.

CASE IV

Two sub-cases must be considered. First, if atom M does not lose TURN % of its initial energy, the treatment used in CASE III will be followed.

Second, if atom M does lose a significant portion of its energy, its velocity components are changed so that the atom is directed back toward the site it occupies. The energy of M is again its initial energy minus the energy gained by the struck atoms. The scale factor used is (Velocity/distance from site). This is multiplied by ΔX , ΔY , and ΔZ to give the velocity components. ΔX is simply the X co-ordinate of the site minus the X co-ordinate of M.

In all cases, atom M's spatial co-ordinates are found by averaging the individual co-ordinates calculated for M in the X, Y, and Z directions (i.e. dividing the sum by NHIT).

If atom M is a primary atom (i.e. one of those considered sequentially for this time step), then the KHIT list is duplicated by the LAST list. Atom M will then proceed to go through its designated collisions, look for more collisions, and go through these until it completes all collisions in this time step.

When atom M has completed all its possible collisions for this time step, each atom that M hit (found in order on the LAST list) undergoes the same process and attempts to hit other atoms. The atoms hit by M, or others on the LAST list, are not inspected for possible further collisions in this time step. We feel that these "secondary" atoms would not have enough time to have a collision in this time step, and if they did, the collisions will be calculated in the next time step. At this point, a possibility does exist that some reasonable collisions are excluded by the process, but extensive calculations have not revealed any examples of this exclusion to date.

The absolute time of an atom's last collision is also calculated during the collision processes described above. For each of the struck atoms this time is the total time from the start of the computation to the start of this time step plus the time, T , of collision (T is measured from the start of the current time step).

The time of M's last collision is taken as the start of its collision with the last atom on the KHIT list (computed as above) plus a certain percentage (PERCENT, an input parameter) of the present time step length. M is thus prevented from participating in further collisions

for a definite period of time after the start of its last collision. We feel that this approach is a valid one, however study of this aspect of the model should be continued to determine its true usefulness.

Sites must now be found for those atoms on the KHIT list whose pre-collision energies were above ETHRESH and whose energies are now below ETHRESH.

If the rounded-off co-ordinates of an atom in this class (call it J) give the co-ordinates of an actual lattice site, then the atom will occupy that site, possibly as part of an interstitial pair if the site is already occupied. Atom J will then be allowed to vibrate around its site until its energy falls below the THERMAL cutoff. If J's rounded-off co-ordinates are not the co-ordinates of a site, then the nearest neighbor sites are found and the site closest, space-wise, to atom J is chosen as J's vibrational center. Again, this may result in the formation of an interstitial pair. Since one of the atoms has an appreciable energy, however, this interstitial pair should be destroyed in the next time step.

The site decided upon may already be occupied by an interstitial pair: if so, a "triple interstitial" is formed. An error counter is then increased (MISTAKE (5)). The possibility of "triple interstitials" could be eliminated by more extensive programming, but an evaluation should first be made of the seriousness of this error. The frequency of formation of these "triple interstitials" has been small thus far, not more than two or three per run, which is tolerable. If this frequency reaches an intolerable level in future development, the model must be modified

to eliminate any possibility of their occurrence.

All atoms on the KHIT list whose post-collision and scaling energies are below THERMAL are placed on the LATER list at this time. Use of the LATER list is discussed below.

If one of the struck atoms on the KHIT list was a member of an interstitial pair, the other atom must now be considered. If this other atom was not hit, and the struck atom now has an energy above ETHRESH (a very unlikely occurrence), then the other atom is placed back on the site, rather than being left in the split interstitial position. We feel that moving the atom back onto the site is more realistic than the definite error of leaving it in the split interstitial position.

All calculations in the model are made on the assumption that the atoms are both space-wise and time-wise at the start of the current time step, except those that have completed the current time step. Therefore, all the atoms on the KHIT list are now moved back in time and space on their post-collision tracks to the start of this time step.

The entire collision process, including the construction of a new NUM list is now repeated for atom M. This repetition will continue for M until M is unable, time-wise, to have further collisions in this time step. The next atom on the LAST list will then become atom M and the collision process will be repeated until this M is unable to have further collisions in this time step. This overall procedure is then repeated until the LAST list has been exhausted.

All the atoms on the LAST list, except those on the LATER list, (the original M is the first atom on the LAST list) are now moved, space and time-wise, to the end of the time step. These atoms have now completed the time step and will not enter into the subsequent calculations until the next time step.

The LATER list is now utilized to place the atoms that have participated in this sequence of collisions and whose energies are below THERMAL on sites, either as members of interstitial pairs or by themselves on previously vacant sites.

The co-ordinates of the atoms on the LAST list are now examined. If an atom has left the lattice, the time step number and the particular face (see APPENDIX I, NFACE) of exit is recorded in the LB array.

This completes the consideration of atom M (the original M) for this time step. The next atom (M + 1) is then considered in the same manner until all atoms have been through the procedure (and, consequently, the time step).

After all the atoms have been through these processes, all unaffected atoms are moved to the end of the time step, which completes the time step. A new time step is then started, or the run is shut down by one of the three processes mentioned earlier.

A numerical example of the order in which atoms are considered may be of some value here. Assume atom #73 (M) hits four atoms simultaneously, atoms 75, 79, 87, and 65. Assume further that #73 hits them in the order: #79, #65, #87, #75. Atom #73 will hit these four, then

repeat the process for further collisions. Assume #73 hits #80 and #67 next, but has no further collisions after that. Then, atom #79 will become the next M since it is second on the LAST list, #65 the next M, and after #75 has completed its possible collisions, if any, the regular sequence will be taken up once more. Atom #73 was the last one considered sequentially, therefore atom #74 now becomes the primary atom, atom M.

As mentioned above, atoms whose energies fall below THERMAL are either placed alone on vacant sites, or formed into split interstitial pairs with other atoms near them. This is done only after a primary atom, together with those on its LAST list, has been completely considered. If this were done at the end of every collision process, it would severely hamper the multiple collision process, and impose a great deal of strain on the credibility of the argument behind it.

When a list of the nearest neighbor sites is formed, if the atom in question (call it MJ) is within one unit of a face of the crystallite, some of the geometrically nearest neighbors normally found will not be present. There are 22 special cases for each one of the two general cases (MJ's co-ordinates are a site or non-site). Sixteen of these special cases for each concern the edges and corners of the crystal. In our model, the 32 (total) possible cases for atom MJ near an edge or corner are not considered separately, but are included in the 12 special cases of when MJ is near a lattice face. When one of the 32 unconsidered special cases does arise, an error counter is increased. Inspection of all

preliminary results to date have, however, shown NO discrepancies as a result of this simplification at the edges and corners of the lattice.

After the list of nearest neighbor sites, the MOON list, is formed, these sites are inspected for possible vacancies. If only one vacancy exists, atom MJ is placed on that site and the appropriate corrections are made to the LB array. If more than one vacancy exists among MJ's nearest neighbor positions, then one of these must be selected for MJ's occupancy. We feel that this selection should be made on a space-wise condition of proximity, rather than on any time-wise condition. Therefore, atom MJ is allowed to occupy the closest vacant site. If there is more than one vacancy at this smallest distance, MJ will be placed on its own site, if available, or the selection will be made in a random manner. The choice of a particular vacancy in the case of multiple vacancies is somewhat unsophisticated, however at this stage of development in the radiation damage field, we feel that no process of a more sophisticated nature can be justified.

If no vacancies exist among atom MJ's nearest neighbor sites, then a prospective interstitial site and partner are chosen. If atom MJ has no energy or velocity, this decision is made on a space-wise basis, i.e. the closest site is chosen. If atom MJ does have energy, then the selection is made on a time-wise basis, i.e. the site that atom MJ passes first.

Once the selection of a prospective interstitial partner has been completed, the atom (call it MM) which occupies the site is found.

Atom MM's nearest neighbor sites are then found, and the list is examined for vacancies. If any vacancies exist, then atom MM is moved to one of these vacant sites by the same method discussed above for MJ. Atom MJ is then moved onto atom MM's recently vacated site and no interstitial is formed.

If, however, atom MM finds no vacancies, then an interstitial pair must be formed. We feel that of the three types of interstitial pairs mentioned earlier, the split interstitial is the most plausible. Indeed, Gibson, et al. have shown the split interstitial to be the only stable configuration.¹⁷ The ΔX , ΔY , and ΔZ distances between atom MJ and the site atom MM occupies are found. The largest of these is taken as the axis of the interstitial pair. Each atom is then placed on its split position, 0.5 units from the site along the axis. Once the appropriate corrections are made to the LB array, the formation of the pair is completed.

7. Operating Procedures

The model consists of three separate but inter-connected programs , MASTER, SLAVE, and RON. Machine memory limitations forced the development of three, rather than one, programs.

The main program, MASTER, is the computational program and does all of the calculations necessary to complete the run. The two secondary programs, SLAVE and RON, merely use the binary output of program MASTER as input and put the results in a semi-analyzed readily legible form. The orbits (or intermediate positions of the moving atoms) are given by program RON while program SLAVE tabulates and categorizes the final positions, energies, etc. of the lattice atoms. Again, because of memory limitations, the two secondary programs may not be combined.

If a binary version of program MASTER is obtained with the FORTBIN compiler, the storage required may be found by listing of the binary tape. The maximum lattice may then be computed. The FORTMAP compiler should be used to compile the large version of MASTER since it requires less memory than the other compilers.

Once program MASTER is compiled, a run may be started. MASTER is called into memory and the run begins. MASTER calls for BCD input on Tape 2, and this is normally transferred to the card reader. BCD output is given on Tapes 3 & 4. Tape 4 is normally transferred to the typewriter for output (see BOX 10, APPENDIX V). The BCD output on Tape 3 is temporary and may be eliminated when the program is working correctly.

This will also make more memory space available .

Program MASTER writes binary output on Tapes 6 , 7 , and 8 . The MASTER output on Tape 6 is the binary input to program RON . The MASTER output on Tape 7 is the regeneration output and is used only by the MASTER program . The MASTER output on Tape 8 is the binary input to program SLAVE . MASTER will automatically rewind each of the three binary tapes when output for a particular tape is completed .

When MASTER has completed computation program SLAVE should be called from our system library . SLAVE calls for BCD input (comment cards , etc.) on Tape 2 , and this is normally transferred to the card reader . SLAVE will then read Tape 8 , compute , and write its BCD output on the designated tape . Program SLAVE , at this time , has PRINT statements for all output except that mentioned in BOX 1 of the SLAVE part of APPENDIX V , and therefore the output will be on Tape 4 unless otherwise directed by the operator .

When SLAVE has completed its run , program RON should be called from the system library . The input and output designations for RON are the same as those for SLAVE except that RON reads Tape 6 rather than Tape 8 .

If , for some reason , MASTER does not complete its run , and Tape 6 is not rewound , program RON must be run with Jump Switch 1 in the set position . This will insure that the correct END designation (in this case a -1) is placed at the end of the information on Tape 6 and that the tape is rewound .

8. Parameter Adjustment

The two input parameters, ETHRESH and TURN primarily govern the cohesiveness or solidity of the lattice. At ETHRESH = 3 ev., for instance, some 400-500 replacements occur with a 100 ev. shot. With ETHRESH raised to 15-25 ev. the number of replacements drops to considerably less than ten, depending on the location and direction of the initial knock-on atom. The best working values seem to lie in the 15-25 ev. range, as preliminary results in this range show good correlation with the work of others. More accurate values of ETHRESH and TURN should be obtained in the future from concurrent N-body calculations for use in the model.

Adjustment of the TURN parameter also governs the length of energy chains. If TURN = 0.0, the energy chains are almost non-existent. Atoms vibrating on their sites are then re-directed toward their sites after their first collision. Since this first collision is usually a slight, glancing one, very little energy is transferred and the energy chain is not seen. If, however, the TURN parameter is set too high, displacements occur among atoms with energy < ETHRESH. Investigations thus far seem to indicate that a value of about 0.1 is the optimum value for TURN.

THERMAL has little effect on the larger aspects of radiation damage i.e. chains, channels, displacements, ring displacement, etc., but has a large effect on machine running time. By changing the value of THERMAL from 0.1 ev. to 0.5 ev., the machine time can be reduced by

75% or more. The very low (below THERMAL) energy vibrations are no longer seen, to be sure, but since this is not one of the areas of primary interest, the advantage of drastically decreased machine time far outweighs the inherent disadvantages.

When the penetration of higher energy (above a few hundred ev.) initial knock-ons is the primary effect under consideration, THERMAL may be set as high as 3-5 ev. For initial knock-on energies of 100 ev. and below, THERMAL should be 0.1 - 0.5 ev. to achieve a reasonable degree of thermalization.

Investigations have shown that the radius of effect (sphere of influence), SPHI, should lie within the range 2.5-2.6 Angstroms (for copper). Values much outside this range (2.2 say) give rather meaningless results. We feel, as a result of the studies we have made, that the best value is probably slightly less than the nearest neighbor distance. For copper, the nearest neighbor distance is $(2)^{1/2}$ (1.807). We have used the value (1.414) (1.807) when not specifically investigating SPHI effects. We feel that any value larger than the nearest neighbor distance will produce invalid results.

Studies of the optimum values for PERCENT and CUTOFF are not completed at this time. Preliminary investigations show that values above 0.1 for PERCENT and below 0.1 for CUTOFF prevent significant collisions from taking place.

The value of TFAC should be kept below 1.0, unless the normal value of 1.0 is used. A more accurate tracing of individual particle

movement is possible with smaller TFAC's, but machine time increases proportionately. A compromise must then be made between the running time available and the individual tracing accuracy desired.

FMASS may be adjusted for the particular metal being used. At present the model is restricted to metals with face centered cubic structure. The Born-Mayer potentials used are restricted to copper only since values of the interaction input parameters (the constants A & B mentioned above) are not available for other materials.

9. Preliminary Results

Preliminary results to date show that the existence of channels, energy and displacement chains, vacancies, interstitials, and replacements depend quite heavily, and quite critically, on the values of the input parameters used. Before very satisfactory results can be obtained, more reliable values of these parameters must be determined.

A run corresponding to Gibson, et al's.¹⁷ Run No. 12 has been made with a slightly modified version of the program, using a 40 ev. primary knock-on. The primary knock-on was shot directly at one of the atoms on the front face (Gibson et al. start their primary knock-on inside the crystallite), at an angle of 15° away from the normal (100) direction.

The values of the various parameters for the run were:

- 1) $IX \times IY \times IZ = 11 \times 15 \times 8$
- 2) ETHRESH = 20.0 ev.
- 3) THERMAL = 0.5 ev.
- 4) CUTOFF = PERCENT = .15 (i.e. 15%)
- 5) SPHI = 2.5
- 6) TFAC = 1.0
- 7) TURN = 0.1

Our results (see Figure 1) are similar to those obtained by Gibson, et al. in that the energy chains play a dominant role in the dissipation of energy. The (100) chain of our run is not as prominent as Gibson, et al's., but strong focusing is observed in the (110) directions. Our (100) chain was terminated prematurely by the velocity turn-around

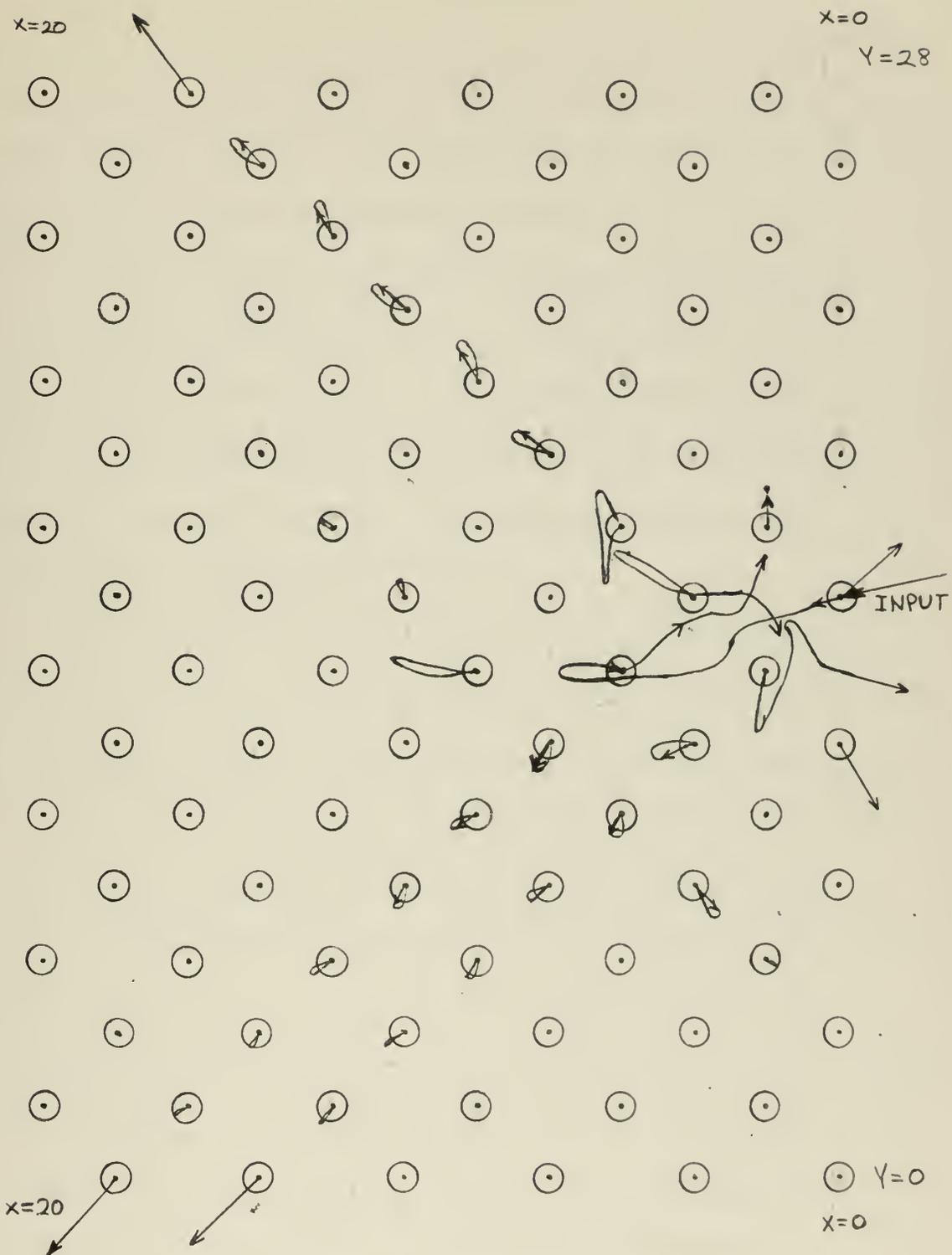


Figure 1. Results of Preliminary Run

mechanism employed for lattice cohesiveness.

10. Recommendations

Many ideas and plans occurred to us during the development of the model to its present level that we have not been able to institute because of time limitations. These unrealized plans and ideas are offered as possible guidelines for future development.

We are convinced at this time that the programming errors in the model are concerned almost wholly with the LB information array. As we did not anticipate the great dependence upon the LB array when we began the problem, we feel that the LB aspects of the entire model (all three programs) must be overhauled, and more orderly storage of the information should be investigated.

Once this overhaul and possible re-arrangement of the LB array has been accomplished and the model is working as designed, a more complete study should be made of the effects of parameter adjustment.

At present when an atom on the LATER list doesn't find a vacancy, a prospective interstitial partner is chosen from the MOON list. A search is then made for vacancies near this partner. If none are found, the interstitial pair is formed. We strongly recommend that when the prospective partner finds no vacancies, the rest of the atoms occupying nearest neighbor sites should also be inspected for vacancies near them. If, again, no vacancies are found then the interstitial pair should be formed between atom MJ and its original prospective partner.

To facilitate this, we recommend that the INVAC subroutine be split into two or more subroutines. There should be a separate

subroutine whose only function is to find the nearest neighbor sites, not necessarily by the present system.

In the present model, if a vacancy occurs near an interstitial pair after the interstitial pair has been formed, this Frenkel pair will not recombine unless the interstitial pair is hit by another atom. Provisions should therefore be made for periodic inspections of all interstitial pairs and any possible vacancies near them. A procedure very similar to that discussed above for making interstitial pairs could be used.

We also feel that subroutines and functions should be incorporated to a much greater extent than at present, and that wider use should be made of comment cards in the programs.

A study of the relative merit of a space-wise versus a time-wise selection process for the KHIT list has been suggested above and should be made.

The ability to use atoms of two different masses should be built into the model. The actual use of two different masses with a Born-Mayer potential must be delayed until appropriate constants for the potential are found.

ETHRESH should be made a directional dependent variable rather than a constant as at present. Since a function able to represent this directional dependence of the displacement energy is not available, a table of thresholds associated with direction seems the most promising course of action.

Two memory saving ideas have occurred to us:

- 1) The possible elimination of the TLAST concept, and
- 2) The possible use of a method, already developed, which packs the co-ordinates and velocity components of an atom into three memory cells rather than the six required at present. This sub-program, SQUEEZE, developed by one of the authors (RLK), saves space at the expense of running time.

The use of these two ideas would save considerable memory space, and enable the users to approximately double the size of the available lattice.

The energy and velocity scaling processes used after the interaction (see BOX 20, APPENDICES III, IV, & V) are a first approximation to the problem and should be considered in that light. We feel that at present this is one of the weakest areas of the model. Considerable effort should be devoted to this section in the future.

11. Conclusions

The model is not fully developed at this time, but we feel that some valid conclusions may be drawn from the results obtained thus far. The MASTER program (see APPENDIX III), as it exists now, still contains some minor programming errors but we feel that the logic is basically sound.

The outstanding attribute of the model at this time seems to be the greatly decreased machine time necessary to achieve results compared to the machine time necessary for an N -body model. This decreased machine time makes it possible to use a lattice as large as the machine memory can accommodate.

We do not feel that this model is sufficiently sophisticated at this time to state definitely the degree of confidence that should be placed in it. We do feel, however, that the preliminary results show that with more work the model can be made into a reasonable approximation to the radiation damage problem. We anticipate that our specific recommendations, if carried out, will lead to a program which approaches this required degree of sophistication.

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APPENDIX I

SPECIFICATION OF UNITS AND ANNOTATED LIST OF VARIABLES

The units used in the model for energy, mass, length, time, and velocity are given below:

ENERGY	The electron volt (ev.), equal to 1.60207×10^{-19} joules.
MASS	The Atomic Mass Unit (AMU), equal to 1.65983×10^{-27} kilograms.
LENGTH	The Angstrom unit, equal to 10^{-10} meters.
TIME	The jiffy, defined as 10^{-14} seconds.
VELOCITY	Derived. One Angstrom/jiffy = 10^4 meters/second.

The variables given below are essentially in the order of their appearance in the program listing. However, certain basic variables are given at the beginning of the list. An asterisk (*) denotes an input variable.

VARIABLE

USAGE

B (I,L)	An array containing the position co-ordinates, velocity components, and energies of the atoms in the lattice. L is the number of the atom. For I there are seven cases: 1 The X co-ordinate in Angstroms 2 The Y co-ordinate in Angstroms 3 The Z co-ordinate in Angstroms 4 The X velocity component in Angstroms/jiffy 5 The Y velocity component in Angstroms/jiffy 6 The Z velocity component in Angstroms/jiffy 7 The energy in electron volts
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VARIABLEUSAGE

LB (L)

An array used for information storage, supplementary to the B array. L is the number of the atom. Stored from right to left we find the following information:

OCTAL

POSITION

MEANING

- | | | |
|---------|-------|--|
| 1 | Bit 1 | 1 if the atom has completed the current time step. |
| | | 0 if the atom has not completed the current time step. |
| | Bit 2 | 1 if the atom has an energy $>$ THERMAL. |
| | | 0 if the atom has an energy \leq THERMAL. |
| | Bit 3 | 1 if the site L is occupied by any atom. |
| | | 0 if the site L is unoccupied. |
| 2-5 | | The number of the time step in which atom L exited the lattice. Zero if L is in the lattice. |
| 6 - 9 | | The number of the other atom in an interstitial pair with atom L. Zero if L is not a member of an interstitial pair. |
| 10 - 13 | | The site occupied by this atom, even if it is the original site. If this number is zero, then the atom has an energy $>$ ETHRESH and is wandering through the lattice. |
| 14 | | The number of the face through which atom L exited the lattice, called NFACE. |

VARIABLEUSAGE

TFAC*	A scaling factor for the Time Step Lengths .
LULL*	The interval, in time steps, at which atoms will be shot into the lattice, provided the proper jump switches are set. Does not affect operation if the jump switches are not set.
IX, IY, IZ*	The X, Y, and Z fixed point dimensions of the lattice, respectively, such as 9 x 14 x 15. IX must be ODD.
A*	One half the side of a unit cell. For copper this is 1,807 Angstroms.
SPHI*	The sphere of influence of an atom. One atom has an SPHI of (1.414)(A), and the other atom is considered to be a point. Given in Angstroms.
ETHRESH*	The displacement threshold energy in electron volts. An atom with an energy $>$ ETHRESH may move through the lattice. Atoms with energy below ETHRESH are forced to remain on their sites in the lattice.
THERMAL*	The thermal energy limit. Atoms with energy above THERMAL are allowed to vibrate on their site. Atoms with energy below THERMAL are placed on sites, or in interstitial pairs by the INVAC subroutine.
FMASS*	The mass of a lattice atom in Atomic Mass Units (AMU).
JPB*	The interval, in time steps, at which the Time Step Length is recalculated.

VARIABLEUSAGE

MNTS*	The maximum number of time steps the program will run.
MNP*	The maximum number of particles to be shot into the lattice.
FI (1-3)	Used throughout the program. Usually denotes the floating point co-ordinates of a particular site.
AB (1-3)	The physical dimensions of the lattice in Angstroms in the X, Y, and Z directions, respectively.
NLINE	The number of atoms in a line in the X direction for the undisturbed lattice.
NPLANE	The number of atoms in any undisturbed X - Y plane of the lattice.
LMAX	The maximum, or total, number of atoms.
MAXLAT	The total number of atoms in the lattice, excluding those shot into the lattice, i.e. the number of sites.
TEMP, TEM	Floating point variables used for temporary storage only.
SITE (L)	A short subroutine. Given the number of a site as an input, SITE computes the fixed point co-ordinates of the site. These are then found in IB (1-3).
TTIME	The total elapsed time from the start of the run to the end of the current time step, in jiffys.
OENERGY	The total original energy of the lattice in ev. This is increased every time a particle is shot into the lattice.

VARIABLEUSAGE

ENERGY	The energy in ev. of the most energetic atom in the lattice. Atoms that have left the lattice are not considered in the computation of ENERGY.
TENERGY	The total energy in ev. in the lattice. This is computed every time step for comparison with OENERGY.
IENERGY	The number of the most energetic atom in the lattice.
MISTAKE (1-10)	An array of 10 error counters. Their meanings are: <ol style="list-style-type: none">1 The number of time steps for which TENERGY varies more than 1% from OENERGY.2 The number of times a vacancy is filled, or an interstitial is formed, near an edge or corner of the lattice.3 The number of times a negative energy was computed.4 The number of times an atom formed an interstitial with itself, i.e. a false interstitial.5 The number of triple interstitials formed.6-9 Not used.10 Set equal to MISTAKE (2) at the start of INVAC so that the increase in MISTAKE (2) may be calculated.
NA	The index for the TSLI and NTSC lists. Always one greater than the number of times the TSL has been recomputed.

VARIABLEUSAGE

NEXT	The number of the next particle to be shot into the lattice. NEXT is one before any atoms are shot into the lattice.
MINTS	The minimum number of time steps, i.e. the lower limit of the time step DO loop. Always one unless the re-generation method is used.
T11	The square of SPHI.
MOVE	An indicator used to determine the exit point from subroutine INVAC.
NOW	The lattice site nearest an atom, computed in INVAC, used to determine an atom's oscillatory center, if the atom's energy is below ETHRESH.
LOCATE	An indicator used to hold the number in Index Register 5, enabling us to use Index Register 5 without destroying the contents.
CON (1-4)	Constants used in the subroutine INTER. These have no relation to the main program.
W (1-4)	Constants used in subroutine INTER. These have no relation to the main program.
XC (1-6)*	Only two used. These are the constant parameters used in the Born-Mayer potential, and can be changed to fit any one of the three types of Born-Mayer for copper, as devised by Gibson, et al. ¹⁷

VARIABLEUSAGE

C1 - C10	Constants used in subroutine INTER. Computed outside the subroutine as a time saving measure.
MASK1 - MASK8	Masking quantities used for logical arithmetic with LB (L). The definition of the significance of the octal positions in LB (L) and the masks themselves explain their specific applicability.
ALFA	10^{-6} A small number for comparison to floating point variables to prevent use of insignificantly small quantities.
ALPHA*	The angle between the original X and Y velocity components of a particle shot into the lattice, given in radians.
BETA*	The angle between the original X and Z velocity components of a particle shot into the lattice, given in radians.
YENTRY (NEXT)	The Y co-ordinate at which a particle shot into the lattice crosses the X = 0 plane. Given in Angstroms.
ZENTRY (NEXT)	The Z co-ordinate at which a particle shot into the lattice crosses the X = 0 plane. Given in Angstroms.
EPB	The energy in ev. of a particle shot into the lattice.
TSL	The Time Step Length in jiffys. TSL is calculated so that the most energetic atom in the lattice will move a distance equal to (TFAC)(A) in one time step.
TSLI (NA)	A list of the first 30 TSL's that are calculated. Used for output purposes only.

VARIABLEUSAGE

NTSC (NA)	A list, corresponding to the TSLI list, that gives the time steps in which the values given in the TSLI table were calculated.
EMAX	A list of the values of ENERGY for the first 30 time steps. Used for output purposes only.
N	The sixth Index Register, and the number of the current time step. The current time step can always be found by stepping the computer console and recording the value of this Index Register. <u>N is used for nothing else.</u>
L	The number of the atom sequentially under consideration. The index of the DO loop starting at Statement 160.
M	The number of the atom currently under primary consideration, usually equal to L.
J	Usually the number of the atom considered in relation to M.
LATER (NZ)	A list of atoms whose energies are less than THERMAL and are to be put through the INVAC subroutine.
NZ	The index for the LATER list, used for no other purpose.
INMIN	The index for the LAST list, used for no other purpose.
INMAX	The maximum number of atoms listed on the LAST list, equal to NMAX when the list is made.
INPUT	An indicator. If zero, then the KHIT list is copied onto the LAST list. If not zero, the LAST list is left untouched.

VARIABLEUSAGE

NUM ()	A list of all the atoms in a box of side length 3.02 (A) centered at atom M. Only atoms on this list are considered as possible targets for M. M is first on the list.
KMAX	The total number of atoms listed on the NUM list.
KHIT ()	A list of atoms, derived from the NUM list, that atom M will hit. Atom M is first on the list.
NMAX	The total number of atoms listed on the KHIT list.
TMIN ()	The time, in jiffys, of closest approach between atom M and the corresponding atom on the NUM list. This assumes no deviation from straight paths. Measured with the start of the current time step as a zero reference.
DSTANCE ()	The distance, in Angstroms, between atoms when at their point of closest approach as determined by their TMIN.
T ()	The time, in jiffys, at which the two atoms are SPHI distance apart. Will be less than the corresponding TMIN if there is to be a collision between M and the atom on the corresponding NUM list.
ITEMP, JTEMP, MTEMP, NTEMP	Fixed point variables used throughout the program for temporary storage purposes. No particular significance.
NPAIR	An indicator for a computed GO TO statement. NPAIR is 3 if one of the atoms being hit is a member of an interstitial pair.

VARIABLEUSAGE

IN3	An indicator that shows the number of those on the NUM list that will be hit by atom M.
LAST ()	A duplicate of the first KHIT list comprised for M when $M = L$. All atoms on the list will become M's when the preceding M is no longer able to have collisions in this time step.
T1 - T10	Temporary variables (see BOX 17, APPENDIX IV) used to speed up computation time.
NFACE	The face of exit of an atom when it leaves the lattice. Faces 1, 3, 5 are the negative X, Y, and Z faces, respectively, while faces 2, 4, 6 are the positive X, Y, and Z faces respectively.
JA	The index for the KHIT list that shows which atom atom M is colliding with at the present time. JA's range is from 2 to NMAX. Has other uses in INVAC.
KMIN	The number on the T list that is smallest. T (KMIN) is the minimum time, and is the collision time for atom NUM (KMIN).
NHIT	The number of atoms on the KHIT list that have been hit by M.
ELOST	The energy in ev. that M lost in its collisions with the other atoms on the KHIT list.

VARIABLEUSAGE

- SAVE (I,K) The pre-collision velocity components and energies of the atoms on the KHIT list. SAVE (1,1) is the initial X velocity of KHIT (1). SAVE (2,1) is the initial Y velocity of KHIT (1), etc. SAVE (4,1) is the energy of KHIT (1).
- COLD () A floating point variable used in the energy and velocity scaling process. COLD (1-6) correspond to the first six co-ordinates in the B array. They are the sums of the individual components of the DEV array after each collision, i.e. COLD (1) is the sum of all the DEV (1,1)'s for a series of collisions. COLD (1) is then the sum of all the X co-ordinates M would have had as a result of the collisions with the rest of the KHIT list.
- PAR The scattering parameters in meters, and the third input to the INTER subroutine.
- TIME The time T for M's previous collision with one of the others on the KHIT list. For instance, if JA is 3, we are considering KHIT (3) in relation to M. TIME is then the T corresponding to KHIT (2).
- DEV (I,1-2) An array, used in subroutine INTER, holding the position co-ordinates, velocities, and energies of the two atoms at the end of the interaction. The first index, I, has the same meaning as the first index of the B array.

VARIABLEUSAGE

The second index is one for atom M, and two for atom J.

The B array is not changed in the subroutine, but the

DEV array contains the output of the subroutine. The

B array is then scaled as necessary.

STUPID

A scale factor used in the velocity scaling process.

SCALE ()

A three member array used in the velocity scaling process.

TURN*

An atom in the intermediate energy range must lose TURN % of its energy before it is re-directed back toward its oscillatory center.

IT

A temporary variable used to facilitate programming. Also the index for the DO loop over the LATER list.

MANY, NANY

The atoms occupying the site chosen for atom M after M's energy has fallen below ETHRESH. If NANY is zero, then M and MANY will become an interstitial pair. If both are non-zero, a "triple interstitial" is formed, while if both are zero, M occupies the site alone.

JPMAX

The number of atoms on the MOON list, i.e. the number of nearest neighbor sites.

MOON ()

A list of nearest neighbor sites for a particular atom.

NOW1, NOW

Temporary variables used to indicate the site chosen as oscillation center for an atom in the intermediate energy range. NOW1 = (NOW shifted 27 binary positions to the left).

VARIABLEUSAGE

NAVY, MAD	Similar to LOCATE, except these are used for Index Registers 2 & 1, respectively.
ZZ (6)	The time in seconds necessary for the interaction.
NN, IL, LL	Variables used to denote atom numbers. NN is the index for the DO loop starting at Statement 241. IL usually denotes a site number, while LL usually denotes the number of the "other" atom in an interstitial pair.
MJ	The number of the atom used as an input to INVAC.
MM	Usually equals MJ, but if MJ finds no vacancies then MM is the prospective interstitial partner atom.
IFACE ()	A three member array denoting the face an atom entering INVAC is near (i.e. within one lattice unit). The index is 1, 2, or 3 for the X, Y, or Z directions, respectively.
NOON ()	The list of vacancies near atom MM (which is usually MJ). This list is derived by examination of the MOON list, i.e. if an atom is not on the MOON list, it will never be on the NOON list.
MAX	Either 1, 2, or 3. Denotes the direction (X, Y, or Z respectively) of the axis of the prospective interstitial pair.

NOTE: This is the end of the list of variables for the MASTER program. Many of the temporary indices are not listed in this table.

The symbols listed below are peculiar to program SLAVE and the usage given applies only to program SLAVE:

<u>VARIABLE</u>	<u>USAGE</u>
NTS	The actual number of time steps the run completed.
KET (1-26)	A list of the energy ranges for the histogram distributions.
IHISTO (1-105)	The histogram format array.
NBUL	The number of knock-ons (i.e. atoms with energy above ETHRESH) in the lattice.
EBUL	The total energy of all knock-ons in the lattice.
NSUBST	The number of replacements in the lattice.
NSAME	The number of atoms on their original lattice sites.
NVAC	The number of vacant lattice sites.
INTERST	The number of interstitial pairs in the lattice.
ETHERM	The total energy of the atoms that have gone through INVAC.
NSIDE (1-6)	The total number of atoms that have left the lattice through each of the six faces.
ESIDE (1-6)	The total energy of the atoms that have left the lattice through each of the six faces.
ECAL	The same as TENERGY, except calculated by Program SLAVE.
LMAXCAL	The same as LMAX, except calculated by Program SLAVE.
YANGLE	Angle ALPHA given in degrees rather than in radians.

<u>VARIABLE</u>	<u>USAGE</u>
ZANGLE	Angle BETA given in degrees rather than in radians .
NUMBERS (1-50)	A fixed point array used for temporary storage only .
IC (1-100)	A fixed point array used for temporary storage of the histogram channels .
DEPTH	The total penetration of an atom in the positive X direction .
PERDIST	The total radial penetration of an atom perpendicular to the X direction .
LL	Usually the number of an atom , temporary usage only .
XYZ (1-3)	Corresponds to the FI array in program MASTER .
NTOTAL	The sum of all the numbers on the NUMBERS list .
NUMBIG	The largest number on the NUMBERS list .
TOTALN	NTOTAL in floating point format .
BIGNUM	NUMBIG in floating point format .

The symbols listed below are peculiar to program RON and the usage given applies only to program RON:

<u>VARIABLE</u>	<u>USAGE</u>
T	Temporary floating point variable . Not to be confused with the T array in program MASTER .
DX	A distance parameter , in Angstroms . If any of an atom's co-ordinates differ from its stored values by DX , the atom's position will be printed , and the new position will be stored .

VARIABLEUSAGE

RA	Reciprocal of A.
P (1-3)	The co-ordinates of the atom under consideration.
IN	The number of the time step the atom under consideration has co-ordinates P (1-3).
X (1-3,N)	Stored co-ordinates of an atom to be written out at a later time.
NT (I)	An array used in the output section. The lower half of a storage cell is the number of the atom whose co-ordinates are X (1-3,N), and the upper half is the time step the atom had these co-ordinates.
NO	An indicator. If greater than zero, a heading has been written on the output tape for the atom under consideration. If less than zero, no heading has been written on the output tape for the atom under consideration.
S (1-3)	Co-ordinates of an atom in floating point form in A units. One A unit is 1.807 Angstroms for copper. (See A, above)

APPENDIX II
LATTICE CONSTRUCTION

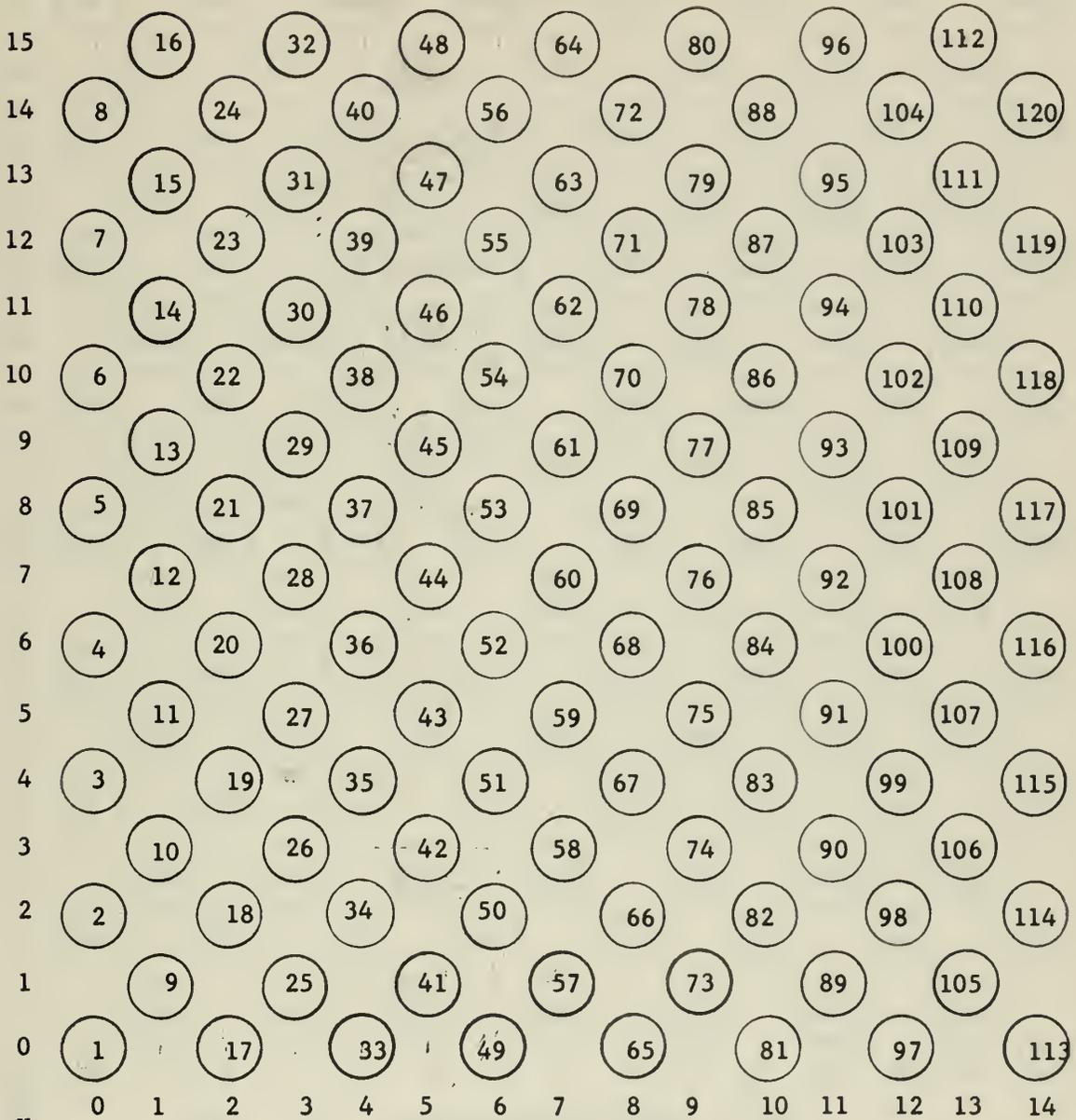


FIG. II (100) LATTICE PLANE, Z EVEN

$IX = 15 \quad IY = 14$

$NLINE = (15+1)/2 = 8$

$NPLANE = (NLINE)(IY+1) = (8)(14+1) = 120$

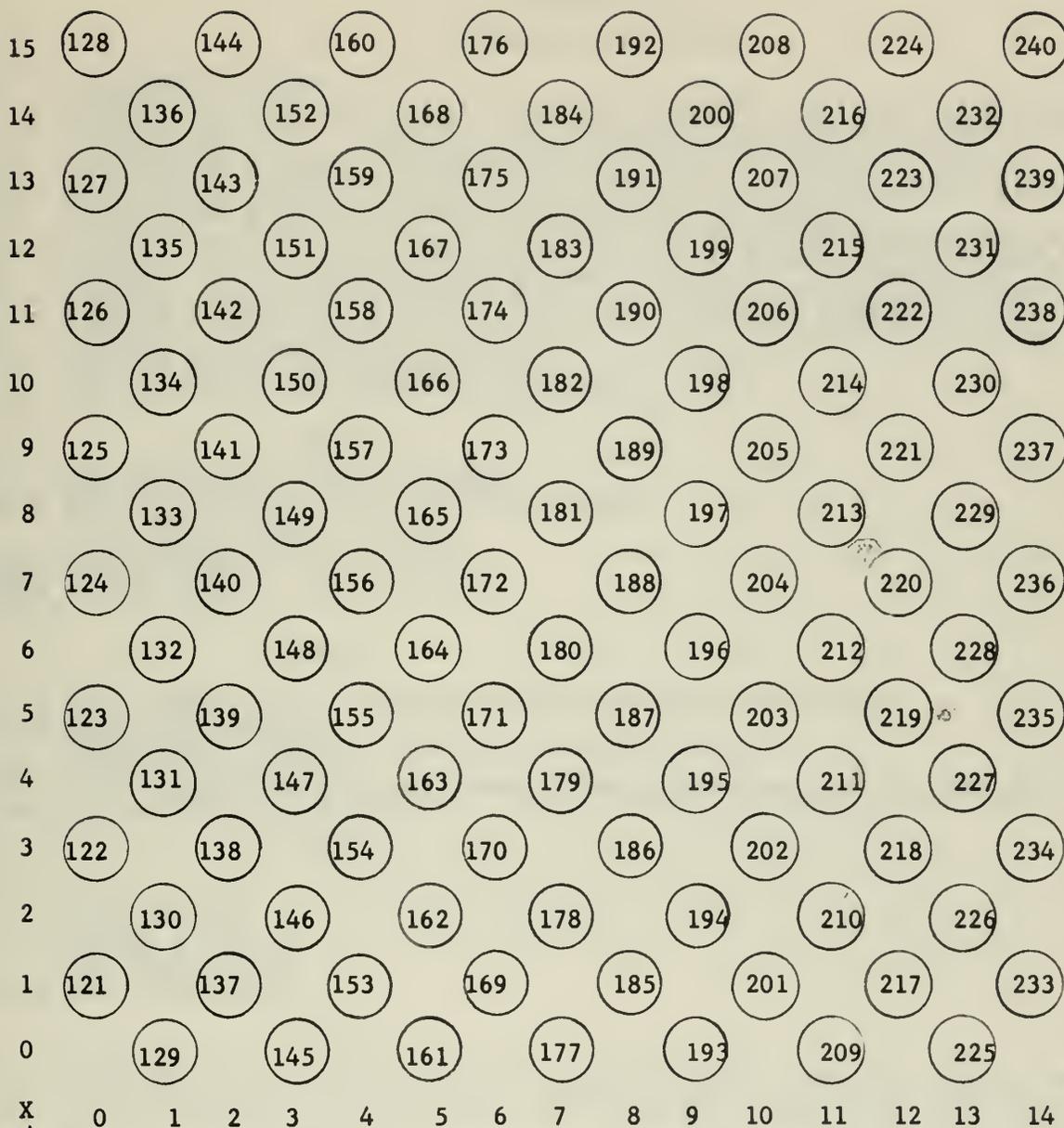


FIG. III (100) LATTICE PLANE, Z ODD

To find the original co-ordinates of atom 77, say:

$$Z = (77-1)/NPLANE = 76/120 = 0 \quad \text{Remainder} = 76$$

$$Y = (76)/NLINE = 76/8 = 9 \quad \text{Remainder} = 4$$

$$X = (4)(2) = 8$$

$$Y + Z = 9 + 0 \quad \text{which is ODD, therefore } X = X + 1 = 9$$

The original co-ordinates of atom 77 were then (7,9,0).

APPENDIX III
PROGRAM LISTINGS

PROGRAM MASTER

```

DIMENSION B(7,1500),LB(1500),OCTAL(1500),FI(3),IB(3),T(20)
DIMENSION TMIN(20),IFACE(3),MISTAKE(10),MOON(15),NOON(10),W(4)
DIMENSION XC(6),XP(20),ZZ(15),CON(4),DEV(7,2),AB(3)
DIMENSION DSTANCE(20),NUM(20),KHIT(20),LATER(50),YENTRY(10)
DIMENSION ZENTRY(10),TSLI(30),NTSC(30),TLAST(1500),LAST(20)
DIMENSION EMAX(30),COLD(7),SAVE(4,10),SCALE(3)
COMMON B,LB,OCTAL,FI,IB,T,TMIN,IFACE,MISTAKE,MOON,NOON,W,XC,XP,ZZ
COMMON CON,DEV,AB,A,NPLANE,NLINE,LMAX,MASK1,MASK2,MASK3,MASK4
COMMON ITEMP,JTEMP,MTEMP,NTEMP,IN2,IN3,IL,JA,JB,JC,JK,JL,JM,JP,JR
COMMON JT,JW,MM,KMIN,MAX,TEMP,NI,JPMAX,NIF,IX,IY,IZ,NN,MAXLAT,JJ
COMMON IP,TE,TEM,C1,C2,C3,C4,C5,C6,C7,C8,C9,C10,C11,C12,T1,T2
COMMON DSTANCE,FMASS,I3,TSL
COMMON MASK5,MASK6,MASK7,MASK8,MOVE,NOW
EQUIVALENCE (XP,TMIN),(LB,OCTAL)

```

BOX 1

```

9950 WRITE OUTPUT TAPE 3,995C
      FORMAT(24H THIS IS PROGRAM MASTER /)
      DO 9980 I=1,5
9980 READ INPUT TAPE 2,9981
9981 WRITE OUTPUT TAPE 3,9981
      FORMAT(80H
1
)

```

BOX 2

```

803 READ INPUT TAPE 2,803,CUTOFF,PERCENT,TFAC,TURN
      FORMAT(4F10.6)
1001 READ INPUT TAPE 2,1001,LLLL,IX,IY,IZ,A
      FORMAT(4I4,F10.6)
102 READ INPUT TAPE 2,102,SPHI,ETHRESH,THERMAL,FMASS,JPR,MNTS,MNP
      FORMAT(4F10.6,3I5)

```

BOX 3

```

      FI(1) = IX
      FI(2) = IY
      FI(3) = IZ
      DO 1000 I=1,3
1000 AB(I)=A*FI(I)

```

BOX 4

```

LDA(IX),INA(1),ENG(0),ARS(1),STA(NLINE),LDA(IY),INA(1),MUI(NLINE)
STA(NPLANE),LDA(IZ),INA(1),MUI(NPLANE),STA(LMAX),STA(MAXLAT)

```

BOX 5

```

      DO 1020 L=1,LMAX
      CALL SITE(L)
1010 DO 1015 I=1,3
      TEMP=IB(I)
1015 B(I,L)=A*TEMP
      ENA4(OB),ALS(27),ADD(48),STA4(LB),LDA(-10.0),STA4(TLAST)
      DO 1020 I=4,7
1020 B(I,L) = 0.0

```

BOX 6

```

WRITE TAPE 6,IX,IY,IZ,AB,MAXLAT,A,SPHI,FMASS,ETHRESH,THERMAL,MNP
WRITE TAPE 6,((B(I,J) I=1,3) J=1,MAXLAT),NLINE,NPLANE
LDA(C.0),STA(TTIME),STA(ENERGY),STA(ENERGY),STA(ZZ+4),ENA(C)
STA(MISTAKE+1),STA(MISTAKE+2),STA(MISTAKE+3),ENA(1),STA(NEXT)
STA(NA),STA(MINTS),LDA(SPHI),FMU(SPHI),STA(T11)
ENA(0),STA(MISTAKE+4),STA(MISTAKE+5),STA(MOVE),STA(NOW)
STA(LOCATE)

```

BOX 7

```

C START SET UP FOR INTERACTION SUBROUTINE
  CON(1)=4.820781099625E-03
  CON(2)=1.089062568935F-01
  CON(3)=4.488872968795E-01
  CON(4)=8.659570911259E-01
  W(1)=0.347854846
  W(2)=0.652145154
  LDA(W+2),STA(W+3),LDA(W+1),STA(W+4)
  READ IN POTENTIAL PARAMETERS
  READ INPUT TAPE 2, 50,(XC(I) I=1,6)
50 FORMAT(10X,6F10.5/)
  C1=1.0E-10*SPHI
  C2=XC(1)*1.6021E-19*EXPF(XC(2))
  C3=XC(2)/C1
  C4=1.6598E-27*FMASS*0.25
  C5=1.0E-14/C1
  C6=0.5E10*C1
  C7=C1*C1
  C8=1.0/C1
  C9=XC(1)*1.6021E-19
  C10=1.0/(FMASS*0.518007615CC)
C END SET UP FOR INTERACTION SUBROUTINE

```

BOXES.8 AND 9

```

MASK1=7777000000B
MASK2=7777000000000000B
MASK3=7777777700000000B
MASK4=7000000000777700B
MASK5=1
MASK6=100000000000000000B
MASK7=2*MASK6
MASK8=7677777777777777B
ALFA=1.0E-6
C USE OF SENSE SWITCHES (SELECTIVE JUMPS)
  UP,UP,UP READ BINARY INPUT OF INTERRUPTED PROGRAM
  UP,UP,DOWN WRITE BINARY CUMP ON TAPE 7 FOR REGENERATION
  UP,DOWN,DOWN READ IN NEXT PARTICLE IF THE TIME IS RIGHT
  DOWN,UP,DOWN JUMP TO 8001 WRITE OUTPUT AND RETURN TO 116
  DOWN,DOWN,UP AT 116, IF SATISFIED,GO ON TO 100, OTHERWISE JUMP TO END,EN
  UP,DOWN,UP WILL WRITE TAPE 8 BINARY, BUT NOT THE BCD PART OF OUTPUT.
  WHILE PRINTING OUTPUT, IF WE PUT STOP SWITCH 1 UP,IT WILL STOP AT THE EN
  OF THE OUTPUT TO ENABLE LS TO RESET THE PROPER SWITCHES,ETC.

```

BOX 10

```

80 SLJ1(80),SLJ(91)
80 SLJ2(81),SLJ(91)
81 SLJ3(90),SLJ(91)
90 READ TAPE 7,MINTS,MNTS,LMAX,B,LB,TLAST,TENERGY,CENERGY,ENERGY,TSL,
  1TSLI,NTSC,TTIME,MISTAKE,YENTRY,ZENTRY,NEXT,NA,EPB,LULL,IX,IY,IZ,A,
  2SPHI,FMASS,JPB,MNP,LAST,EMAX,VMOM,COLD,EFOUND
  REWIND 7
91 DO 9000 N=MINTS,MNTS
  WRITE OUTPUT TAPE 3,8100,TENERGY,N,IENERGY,ENERGY
  WRITE OUTPUT TAPE 4,8100,TENERGY,N,IENERGY,ENERGY
8100 FORMAT(F15.9,2I8,F15.9)
  IENERGY=0
  THIS IS THE START OF THE MAIN DO LOOP OF THE PROGRAM, THE ONE ON TIME
  STEPS. WE CAN CHECK THE CURRENT TIME STEP BY STEPPING THE 1604 AND
  NOTING THE CONTENTS OF INDEX REGISTER 6.
  SLJ1(82),SLJ(93)
82 SLJ2(83),SLJ(93)
83 SLJ3(93)
92 WRITE TAPE 7,N,MNTS,LMAX,B,LB,TLAST,TENERGY,CENERGY,ENERGY,TSL,
  1TSLI,NTSC,TTIME,MISTAKE,YENTRY,ZENTRY,NEXT,NA,EPB,LULL,IX,IY,IZ,
  2A,SPHI,FMASS,JPB,MNP,LAST,EMAX,VMOM,COLD,EFOUND
  REWIND 7
93 CONTINUE

```

BOX 11

```

      SLJ1(100),SLJ2(85),SLJ(100)
85  SLJ3(100),SLJ(8001)
116 SLJ1(9999),SLJ2(9999),SLJ3(100),SLJ(9999)
100 LDA(NEXT),INA(-1),AJP(120),SLJ1(84),SLJ(110)
84  SLJ2(110),SLJ3(110),SLJ(115)
110 LDA(ENERGY),FSB(THERMAL),AJP(8001),AJP2(130),SLJ(8001)
115 ENA6(18),DVI(LULL),QJP1(130),LDA(NEXT),SUB(MNP),AJP(120),AJP2(130)
120 RAO(LMAX),LIL1(LMAX),ENA(2),STA1(LB),LDA(-2.0),STA1(TLAST)
900 READ INPUT TAPE 2,500,(B(I,LMAX) I=1,3),B(7,LMAX),ALPHA,BETA
500 FORMAT(6F10.6)
      YENTRY(NEXT)=B(2,LMAX)
      ZENTRY(NEXT)=B(3,LMAX)
      RAO(NEXT)
      ZZ(1)=TANF(ALPHA)
      FMU(ZZ+1) STA(ZZ+2)
      ZZ(3)=TANF(BETA)
      FMU(ZZ+3) FAC(ZZ+2) FAC(1.0) STA(ZZ+2)
      B(4,LMAX)=SQRTF(B(7,LMAX)*C10/ZZ(2))
      B(5,LMAX)=B(4,LMAX)*ZZ(1)
      B(6,LMAX)=B(4,LMAX)*ZZ(3)
      B(3,LMAX)=B(3,LMAX)-B(6,LMAX)/B(4,LMAX)
      B(2,LMAX)=B(2,LMAX)-B(5,LMAX)/B(4,LMAX)
125  OENERGY=OENERGY+B(7,LMAX)
      TENERGY=TENERGY+B(7,LMAX)
      EPB=B(7,LMAX)
      TSL=A*0.7197274588/SQRTF(ABSF(B(7,LMAX)/FMASS))*TFAC
      +LDA(NA),INA(-30),+AJP(L+1),AJP2(140),LIL1(NA),LDA(TSL)
      STA1(TSLI),ENA6(0),STA1(NTSC),RAC(NA),SLJ(140)

```

BOX 12

```

130 ENA6(0),ENQ(0),DVI(JPB),CJP1(140)
135 TSL=A*0.7197274588/SQRTF(ABSF(ENERGY/FMASS))*TFAC
      +LDA(NA),INA(-30),+AJP(L+1),AJP2(140)
      LIL1(NA),LDA(TSL),STA1(TSLI),ENA6(0),STA1(NTSC),RAO(NA)

```

BOX 13

```

140 LDA(TTIME),FAD(TSL),STA(TTIME)
      LDA(OENERGY),FMU(1.01),FSB(TENERGY),AJP(155),AJP3(150),LDA(O.C)
      FSB(OENERGY),FMU(0.99),FAD(TENERGY),AJP(155),AJP2(155)
150 RAO(MISTAKE+1)

```

BOX 14

```

155 ENA6(0),INA(-31),+AJP2(L+3),LDA(ENERGY),INI6(-1),STA6(EMAX)
      +INI6(1),+LDA(0.0),STA(ENERGY),STA(TENERGY)
      DO 160 L=1,LMAX
      TENERGY=TENERGY+B(7,L)
      +LDA4(LB),SCL(MASK5),STA4(LB)
160 CONTINUE

```

BOX 15

```

C THIS IS THE START OF THE MAJOR DO LOOP ON THE PARTICLES
C DO 8000 L=1,LMAX
C WITHIN A PARTICULAR TIME STEP, THIS IS THE START OF THE MAIN DO LOOP ON
C ALL THE PARTICLES IN THE LATTICE. WE CAN TELL WHICH PARTICLE IS BEING
C SIDERED BY STEPPING THE 16C4 AND CHECKING INDEX REGISTER 4.
      LDQ4(LB),LDL(2B),AJP(8000),LDL(77771B),AJP1(8000)
      LDL(MASK7),AJP1(8000)
165 DO 161 K=1,50
161  LATER(K)=0
      ENA(1),STA(NZ),ENA(2),STA(INMIN),ENA(0),STA(INPUT)
      DO 164 K=1,20
      ENA(0),STA3(NUM),STA3(KHIT),STA3(LAST),LDA(0.0),STA3(T)
      STA3(DSTANCE),STA3(TMIN)
164 CONTINUE
      SIL4(ITEMP),LIL5(ITEMP)
C THIS IS THE END OF THE USE OF L AS SUCH FOR THE REST OF THE DO LOOP

```

BOX 16

```

200 ENA(C),STA(IN3),ENAS(0),AJP(277),ENI3(2),SIL5(NUM+1),SIL5(KHIT+1)
LDQ5(LB),LDL(MASK7),AJP1(277)
NPAIR=1
DO 201 I=1,3
201 T(I)=B(I,M)
DO 203 J=1,LMAX
LDQ2(LB),LDL(77771B),AJP1(203)
DO 202 I=1,3
IF(ABSFB(I,J)-T(I))-1.51*A 202,203,203
202 CONTINUE
SIL2(ITEMP),LAC(ITEMP),INA5(0),AJP(203),ENA2(0),STA3(NUM),INI3(1)
203 CONTINUE
INI3(-1),ENA3(0),STA(KMAX),INA(-2),AJP3(277),ENA(0),STA(IN3)
STA(NFACE)

```

BOX 17

```

DO 215 K=1,KMAX
LDA3(NUM),STA(ITEMP)
T1=B(1,ITEMP)-B(1,M)
T2=B(2,ITEMP)-B(2,M)
T3=B(3,ITEMP)-B(3,M)
T4=B(4,ITEMP)-B(4,M)
T5=B(5,ITEMP)-B(5,M)
T6=B(6,ITEMP)-B(6,M)
T7=T4*T4+T5*T5+T6*T6
T8=T1*T1+T2*T2+T3*T3
LDA(T7),FSB(ALFA),AJP3(214)
T9=T1*T4+T2*T5+T3*T6
LDA(1.0),FDV(T7),STA(T10),LAC(T9),FMU(T10),STA3(TMIN)
DSTANCE(K)=SQRTF(ABSFB(T1+T4*TMIN(K))*(T1+T4*TMIN(K))+(T2+T5*TMIN(
1K))*(T2+T5*TMIN(K))+(T3+T6*TMIN(K))*(T3+T6*TMIN(K))))
FSB(SPHI),AJP(214),AJP2(214)
T(K)=TMIN(K)-SQRTF(ABSFB(TMIN(K)*TMIN(K)-(T8-T11)/T7))
211 LDA3(T),FSB(TSL),AJP(214),AJP2(214),FAC(TSL),FAC(TSL),AJP3(214)
LDA3(T),FDV(TSL),FSB(0.95999),AJP(212),AJP2(214)
212 LIL1(ITEMP),LDA3(T),FAD(TTIME),FSB(TSL),FSB1(TLAST),AJP(214)
AJP3(214),LDA3(T),FAD(TTIME),FSB(TSL),FSB5(TLAST),AJP(214)
AJP3(214)
213 RAO(IN3),SLJ(215)
214 LDA(TSL),FMU(1.0E+2),STA3(T)
215 CONTINUE

```

BOX 18

```

LDA(IN3),AJP1(216),SLJ(277)
216 LDA(KMAX),INA(-1),STA(JA),LDA(TSL),FMU(1.0E+3),STA(TEMP)
DO 217 K=2,KMAX
LDA3(T),FSB(TEMP),AJP2(217),LDA3(T),STA(TEMP),SIL3(KMIN)
217 CONTINUE
LIL1(KMIN),ENI2(2),LDA(TSL),FMU(CUTOFF),STA(T1)
DO 219 K=1,KMAX
LDA3(T),FSB1(T),FSB(T1),AJP(218),AJP2(219)
218 LDA3(NUM),STA2(KHIT),INI2(1)
219 CONTINUE
INI2(-1),SIL2(NMAX),LDA(INPUT),AJP1(301),SIL2(INMAX)
DO 300 K=1,INMAX
LDA3(KHIT),STA3(LAST)
300 CONTINUE
301 RAO(INPUT),LDA(NMAX),INA(-1),AJP1(220),SLJ(277)
220 ENA(2),STA(JA),ENA(0),STA(NHIT),LDA(0.0),STA(ELCST)

```

BOX 19

```

DO 351 K=1,NMAX
J=KHIT(K)
DO 351 I=1,4
351 SAVE(I,K)=B(I+3,J)
DO 430 I=1,7
430 COLD(I)=0.0
221 J=KHIT(JA)
224 LDQ2(LB),LDL(MASK1),+AJP(L+2),ENA(3),-STA(NPAIR)
DO 245 K=1,KMAX
LAC3(NUM),INA2(0),AJP(246)
245 CONTINUE
246 PAR=DSTANCE(K)*1.0E-10
DO 240 I=1,3
B(I,J)=B(I,J)+B(I+3,J)*T(K)
LDA(JA),INA(-2),AJP(225)
B(I,M)=B(I,M)+B(I+3,M)*(T(K)-TIME)
SLJ(240)
225 B(I,M)=B(I,M)+B(I+3,M)*T(K)
240 CONTINUE
TIME=T(K)
LDA2(LB),SCL(MASK7),STA2(LB)
380 CALL INTER(M,J,PAR)
TLAST(J)=TTIME-TSL+TIME
805 DO 227 I=1,7
COLD(I)=COLD(I)+DEV(I,1)
227 B(I,J)=DEV(I,2)
COLD(7)=0.0
ELOST=B(7,J)-SAVE(4,JA)+ELCST
SLJ(221)

```

BOX 20

```

T2=B(7,M)-ELOST
AJP(356),AJP2(229),LDA(0.0),STA(TEMP),STA(TEM)
356 DO 357 I=4,7
357 B(I,M)=0.0
LDA(T2),AJP(229)
DO 358 K=1,NMAX
J=KHIT(K)
520 DO 352 I=1,3
TEMP=TEMP+SAVE(I,K)*SAVE(I,K)
TEM=TEM+B(I+3,J)*B(I+3,J)
352 CONTINUE
358 CONTINUE
TEMP=TEMP/TEM
STUPID=SQRTF(ABSF(TEMP))
DO 355 K=2,NMAX
J=KHIT(K)
521 DO 354 I=4,6
354 B(I,J)=STUPID*B(I,J)
B(7,J)=B(7,J)*TEMP
355 CONTINUE
229 TEM=NHIT
TEM=1.0/TEM
DO 359 I=1,3
359 B(I,M)=COLD(I)*TEM
LDA(T2),AJP(231),AJP3(231),LDA(SAVE+4),FSB(ETHRESH),AJP2(503)
LAC(SAVE+4),FMU(TURN),FAD(ELOST),AJP(L+2),AJP2(L+1),SLJ(503)
LDQ5(LB),LDL(MASK2),ARS(27),STA(IL),LDA(0.0),STA(TEM)
CALL SITE(IL)
DO 501 I=1,3
TEMP=IB(I)
SCALE(I)=TEMP*A-B(I,M)
FMU1(SCALE),FAD(TEM),STA(TEM)
501 CONTINUE
LDA(TEM),FSB(ALFA),AJP(503),AJP3(503)
TEM=SQRTF(ABSF(T2*C10/TEM))
DO 502 I=1,3
502 B(I+3,M)=TEM*SCALE(I)
B(7,M)=T2
GO TO 231
503 LDA(NHIT),INA(-1),AJP1(505)
DO 504 I=4,7
504 B(I,M)=DEV(I,1)
GO TO 231
505 TEMP=0.0
DO 329 I=4,6
LDA1(COLD),FMU1(COLD),FAC(TEMP),STA(TEMP)
329 CONTINUE
B(7,M)=T2
TEMP=SQRTF(ABSF(C10*B(7,M)/TEMP))
230 B(I,M)=COLD(I)*TEMP

```

BOX 21

```

231 ENA(O), STA(NX), STA(NY), +LDA(NHIT), AJP1(L+2), STA(IN3), SLJ(277)
    TLAST(M)=TTIME-TSL+TIME+TSL*PERCENT
    LOCATE=0
    TEMP=B(7,M)
    FSB(ETHRESH), AJP(L+9), +AJP3(L+8), LDQ(MASK2), LCL5(LB), AJP(L+4)
    +ARS(3), STA(ITEMP), LIU1(ITEMP), LDA1(LB), SCL(4B), STA1(LB), LDA5(LB)
    SCL(MASK2), SST(2B), STA5(LB), +SLJ(514), +LDA(TEMP), FSB(THERMAL)
    AJP2(L+1), SLJ(L+3), LDQ(MASK2), LDL5(LB), AJP1(513), SLJ(L+23)
    +LDA5(LB), +SCL(2B), STA5(LB), LDQ(MASK2), STL(ITEMP)
    LDQ(MASK1), STL(JTEMP), LDA(JTEMP), AJP1(L+6), +LDA(ITEMP), AJP(L+4)
    ARS(27), STA(ITEMP), LIL1(ITEMP), LDA1(LB), SCL(4B), STA1(LB), SLJ(L+4)
    +ARS(15), STA(JTEMP), LIL1(JTEMP), LDA1(LB), SCL(MASK1), STA1(LB)
    LDA5(LB), SCL(MASK3), LDQ(MASK6), STL(ITEMP), SCL(MASK6), STA5(LP)
    LDA(ITEMP), AJP1(L+4), LIL1(NZ), ENA5(O), STA1(LATER), INI1(1)
    +SIL1(NZ), +LDA(TEMP), AJP(L+2), AJP2(L+1), RAO(MISTAKE+3), ENA(C)
    STA(LOCATE)
600 SIL5(MJ), ENA(1), STA(MOVE), ENA(O), STA(NCW)
    CALL INVAC(MJ)
    ENA(C), STA(MOVE), LDA5(LB), SCL(MASK7), STA5(LP), LDQ(NOW), QJP(510)
    QLS(27), STQ(NOW1)
509 LDA5(LB), SSU(MASK2), STA5(LB), LIL1(NOW), LDQ1(LB), LDL(4B), AJP1(L+3)
    -LDA1(LB), SST(4B), STA1(LB), SLJ(513), +ENA(O), STA(MANY), STA(NANY)
    DO 507 I=1, LMAX
    LDQ1(LB), LDL(MASK2), SUB(NCW1), AJP1(507), LDL(MASK1), AJP(508)
    ARS(15), STA(MANY), LDQ(NANY), QJP1(507), STA(NANY)
507 CONTINUE
508 ENA1(O), AJP1(L+4), +LIL1(NOW), LDA1(LB), SCL(4B), STA1(LB), LCC(NOW1)
    SLJ(509), LDA(MANY), SUB(NANY), +AJP1(L+1), RAO(MISTAKE+5), LDA(NANY)
    ALS(15), STA(ITEMP), ENA5(C), ALS(15), STA(JTEMP), LDA5(LB), LDQ(MASK1)
    SSU(ITEMP), STA5(LB), +LIL1(NANY), +LDA1(LB), SSU(JTEMP), STA1(LB)
    ENA1(O), SUB(MANY), AJP(513), LIL1(MANY), SLJ(L-3)
510 DO 511 K=1, JPMAX
    LDA3(MOON), STA(IL), LDA(O.C), STA3(DSTANCE)
    CALL SITE(IL)
    DO 511 I=1, 3
    TEMP=IB(I)
    TEMP=B(I,M)-TEMP*A
511 DSTANCE(K)=DSTANCE(K)+TEMP*TEMP
    I=1
    DO 512 K=2, JPMAX
    LDA3(DSTANCE), FSB1(DSTANCE), AJP3(L+1), SLJ(512), SIL3(IT), LIL1(IT)
512 CONTINUE
    LDQ1(MOON), STQ(NOW), QLS(27), STQ(NOW1), SLJ(509)
    LDA(LOCATE), AJP1(516), LDA(T2), AJP(L+2), AJP2(L+1), RAO(MISTAKE+3)

```

BOX 22

```

514 ENI1(2)
515 LDA1(KHIT),STA(IT),LIL2(IT)
      T1=B(7,J)
      FSB(ETHRESH),AJP(L+9),+AJP3(L+8),LDQ(MASK2),LDA2(LB),STL(ITEMP)
      SCL(MASK2),SST(2B),STA2(LB),LDA(ITEMP),AJP(233),ARS(3),LIU3(ITEMP)
      LDA3(LB),SCL(4B),STA3(LB),+SLJ(233),+LDA(T1),FSB(THERMAL)
      AJP(L+1),AJP2(L+17),LDQ(MASK2),LDA2(LB),SCL(2B),STA2(LB)
      STL(ITEMP),LDQ(MASK1),STL(JTEMP),LDA(JTEMP),AJP(L+8),ARS(15)
      STA(JTEMP),LIL3(JTEMP),LCA3(LB),SCL(MASK1),STA3(LB),LDA2(LB)
      SCL(MASK3),SST(MASK6),STA2(LB),LIL3(NZ),ENA2(O),STA3(LATER)
      RAO(NZ),SLJ(233),LDA(ITEMP),ARS(27),STA(ITEMP),LIL3(ITEMP)
      LDA3(LB),SCL(4B),+SLJ(L-8),+LDQ(MASK2),LDA2(LB),SST(2B),STA2(LB)
      LDL2(LB),AJP1(233),SIL5(LOCATE),SIL2(NAVY),LIL5(NAVY),SIL1(MAD)
      SLJ(600)
516 LIL2(NAVY),LIL5(LOCATE),LIL1(MAD)
233 ENA1(O),SUB(NMAX),AJP(234),INI1(1),SLJ(515)

```

BOX 23

```

234 LDA(NHIT),AJP1(241),LDA(C.O),STA(ZZ+6),SLJ(283)
241 DO 282 NN=1,NMAX
      J=KHIT(NN)
      DO 280 K=1,KMAX
      LAC3(NUM),INA2(O),AJP(281)
280 CONTINUE
281 LDA(NN),INA(-1),+AJP(L+2),LDA3(T),-STA(TIME)
      DO 235 I=1,3
235 B(I,J)=B(I,J)-(TIME+ZZ(6)*1.0E+14)*B(I+3,J)
282 CONTINUE

```

BOX 24

```

283 GO TO (277,277,236,277),NPAIR
236 DO 238 K=2,NMAX
      J=KHIT(K)
      T2=B(7,J)
      FSB(ETHRESH),AJP(526),AJP3(526),LDQ2(LB),LDL(MASK2),AJP(238)
      STA(IL),LDL(MASK1),AJP(238),STA(LL),LDA2(LB),SCL(MASK3),STA2(LB)
      LDA(LL),ARS(15),STA(LL)
      T4=B(7,LL)
      FSB(ETHRESH),AJP3(L+7),LIL1(LL),LDA1(LB),SCL(MASK3),STA1(LB)
      LDA(IL),ARS(3),STA(IL),LIU1(IL),LDA1(LB),SCL(4B),STA1(LB),SLJ(238)
      LIL1(LL),LDA1(LB),SCL(MASK1),STA1(LB),LDQ(MASK7),STL(IT),LDA(IT)
      AJP(238),LDA(IL),ARS(27),+STA(IL)
      CALL SITE(IL)
      DO 237 I=1,3
      TEMP=IB(I)
237 B(I,LL)=A*TEMP
      GO TO 238
526 LDQ2(LB),LDL(MASK1),AJP(238),ARS(15),STA(LL),LIL1(LL)
      T4=B(7,LL)
      FSB(ETHRESH),AJP3(238),LCA1(LB),SCL(MASK3),STA1(LB),LDA2(LB)
      SCL(MASK1),STA2(LB)
238 CONTINUE

```

BOX 25

```

277 LDA(IN3),AJP1(200),LDA(INMIN),SUB(INMAX),AJP(302),AJP2(303)
302 M=LAST(INMIN)
      RAO(INMIN),LDQ5(LB),LDL(MASK6),AJP1(277),SLJ(200)

```

BOX 26

```

303 DO 305 J=1, INMAX
      K=LAST(J)
      LDQ3(LB), LDL(MASK6), AJP1(525)
      DO 304 I=1, 3
304  B(I,K)=B(I,K)+B(I+3,K)*TSL
      LDA3(LB), SST(18), STA3(LB)
525  IF(ENERGY-B(7,K)) 350,305,305
350  ENERGY=B(7,K)
      IENERGY=K
305  CONTINUE

```

BOX 27

```

      LDA(NZ), INA(-1), AJP(262), AJP3(262), STA(IT1)
      DO 261 IT=1, IT1
      MJ=LATER(IT)
      CALL INVAC(MJ)
      ENA(0), STA(IU), SIU6(IU) LDA(MJ) RAD(IU)
      WRITE TAPE 6, IU, (B(I,MJ) I=1,3)
261  CONTINUE

```

BOX 28

```

262 DO 7998 J=1, INMAX
      LDA2(LAST), STA(ITEMP), LIL5(ITEMP), LDQ5(LB), LDL(MASK7), AJP1(7999)
250 DO 252 I=1, 3
      IF(B(I,M)-AB(I)) 251,251,254
251  IF(B(I,M)) 255,252,252
252  CONTINUE
      GO TO 307
254  ENA(0), ALS(1), STA(NFACE), SLJ(252)
255  ENA(0), ALS(1), INA(-1), STA(NFACE), SLJ(252)
307  LDA(NFACE), AJP(7998), ALS(36), INA6(0), ALS(3), STA(ITEMP), LDA5(LB)
      LDQ(MASK4), SSU(ITEMP), LDC(MASK2), STL(ITEMP), LDQ(MASK1), STL(JTEMP)
      SCL(MASK3), STA5(LB), ENA(C), STA(NFACE), LDA(JTEMP), AJP1(331)
      LDA(ITEMP), ARS(27), STA(ITEMP), LIL1(ITEMP), LDA1(LB), SCL(4B)
      STA1(LB), SLJ(7998)
331  ARS(15), STA(JTEMP), LIL1(JTEMP), LDA1(LB), SCL(MASK1), STA1(LB)
7998 CONTINUE
8000 CONTINUE
C THIS IS THE END OF THE MAJOR DO LOOP ON THE PARTICLES

```

BOX 29

```

      ENA(0), STA(IT), SIU6(IT)
      DO 9000 L=1, LMAX
      LDQ4(LB), LDL(2B), AJP(309), SIL4(IT)
      WRITE TAPE 6, IT, (B(I,L) I=1,3)
309  LDQ4(LB), LDA(MASK8), STL4(LB), LDL(77771B), AJP1(9000)
      LDL(MASK7), AJP1(320)
      DO 310 I=1, 3
310  B(I,L)=B(I,L)+B(I+3,L)*TSL
      DO 312 I=1, 3
      IF(B(I,L)-AB(I)) 311,311,314
311  IF(B(I,L)) 315,312,312
312  CONTINUE
      GO TO 257
314  ENA(0), ALS(1), STA(NFACE), SLJ(312)
315  ENA(0), ALS(1), INA(-1), STA(NFACE), SLJ(312)
257  LDA(NFACE), AJP(320), ALS(36), INA6(0), ALS(3), STA(ITEMP), LDA4(LB)
      LDQ(MASK4), SSU(ITEMP), LDC(MASK2), STL(ITEMP), LDQ(MASK1), STL(JTEMP)
      SCL(MASK3), STA4(LB), ENA(C), STA(NFACE), LDA(JTEMP), AJP1(332)
      LDA(ITEMP), ARS(27), STA(ITEMP), LIL1(ITEMP), LDA1(LB), SCL(4B)
      STA1(LB), SLJ(320)
332  ARS(15), STA(JTEMP), LIL1(JTEMP), LDA1(LB), SCL(MASK1), STA1(LB)
320  IF(ENERGY-B(7,L)) 316,9000,9000
316  ENERGY=B(7,L)
      IENERGY=L
9000 CONTINUE
C THIS IS THE END OF THE MAJOR DC LOOP ON THE TIME STEPS

```

```

8001 WRITE TAPE 8, IX, IY, IZ, AB, NLINE, NPLANE, MAXLAT, LMAX, A, SPHI, FMASS,
1ETHRESH, THERMAL, EPB, LULL, ALPHA, BETA, N, MNTS, TTIME, TSLI, NTSC,
20ENERGY, TENERGY, MISTAKE, YENTRY, ZENTRY, NA, EMAX, EFOUND
WRITE TAPE 8, (LB(L), (B(I, L) I=1, 7) L=1, LMAX)
REWIND 8
+SL S1(L+1), +SLJ1(L+1), SLJ(L+2), SLJ2(L+1), SLJ3(9998)
WRITE OUTPUT TAPE 3, 9951, TTIME
9951 FORMAT(1H1, 19H THE TOTAL TIME IS F13.7, 7H JIFFYS )
WRITE OUTPUT TAPE 3, 9952, TSL
9952 FORMAT(25H THE TIME STEP LENGTH IS F13.7, 7H JIFFYS)
IF(N) 9974, 9974, 9973
9973 WRITE OUTPUT TAPE 3, 9953, ENERGY, N
GO TO 9972
9974 WRITE OUTPUT TAPE 3, 9953, ENERGY, MNTS
99530 FORMAT(9H ENERGY= F15.7, 15H ELECTRON VOLTS/14, 27H TIME STEPS HAV
1E BEEN TAKEN )
9972 WRITE OUTPUT TAPE 3, 9954, TENERGY, OENERGY
99540 FORMAT(21H THE TOTAL ENERGY IS F12.7, 15H ELECTRON VOLTS/24H THE C
1RIGINAL ENERGY IS F12.7, 15H ELECTRON VOLTS)
IF(MISTAKE(1)) 9955, 9955, 9956
9955 WRITE OUTPUT TAPE 3, 9957
9957 FORMAT(30H THE ENERGY CHECK DID NOT FAIL )
GO TO 9965
9956 WRITE OUTPUT TAPE 3, 9959, MISTAKE(1)
9959 FORMAT(24H THE ENERGY CHECK FAILED 14, 16H DIFFERENT TIMES)
9965 IF(MISTAKE(2)) 9961, 9961, 9962
9961 WRITE OUTPUT TAPE 3, 9963
9963 FORMAT(62H NO INTERSTITIALS OR VACANCIES OCCURED ALONG AN EDGE OR
1CORNER )
GO TO 9805
9962 WRITE OUTPUT TAPE 3, 9960, MISTAKE(2)
9960 FORMAT(60H AN INTERSTITIAL CR VACANCY OCCURRED ALONG AN EDGE CR CO
1RNER 14, 16H DIFFERENT TIMES)
9805 IF(MISTAKE(3)) 9800, 9800, 9801
9800 WRITE OUTPUT TAPE 3, 9803
9803 FORMAT(36H NO NEGATIVE ENERGIES WERE COMPUTED /)
GO TO 107
9801 WRITE OUTPUT TAPE 3, 9804, MISTAKE(3)
9804 FORMAT(31H A NEGATIVE ENERGY WAS COMPUTED 14, 16H DIFFERENT TIMES
1 /)
107 IF(MISTAKE(4)) 170, 170, 172
170 WRITE OUTPUT TAPE 3, 171
171 FORMAT(37H NO FALSE INTERSTITIALS WERE FORMED /)
GO TO 174
172 WRITE OUTPUT TAPE 3, 173, MISTAKE(4)
173 FORMAT(13, 34H FALSE INTERSTITIALS WERE FORMED /)
174 WRITE OUTPUT TAPE 3, 175, MISTAKE(5)
175 FORMAT(10H WE FORMED 14, 22H TRIPLE INTERSTITIALS )
WRITE OUTPUT TAPE 3, 108, IX, IY, IZ
1080 FORMAT(35H THE DIMENSIONS OF THE LATTICE ARE //13H X DIRECTION
112, 7H UNITS /13H Y DIRECTION 12, 7H UNITS /13H Z DIRECTION
212, 7H UNITS )
WRITE OUTPUT TAPE 3, 106
106 FORMAT(87H L X Y Z VX VY
1 VZ E LB(L)/)
DO 1025 L = 1, LMAX
1025 WRITE OUTPUT TAPE 3, 103, L, (B(I, L) I=1, 7), OCTAL(L)
103 FORMAT(1X, 14, 7F10.4, 019)
9998 ENA6(0), AJP(9990), SLS1(116)
9990 WRITE OUTPUT TAPE 3, 9991
9991 FORMAT(/// 32H THE RUN WENT THE FULL DISTANCE )
9999 JT=-1
WRITE TAPE 6, JT
REWIND 6
END

```

BOX 31

```

SUBROUTINE SITE(M)
DIMENSION B(7,1500),LB(1500),OCTAL(1500),FI(3),IB(3),T(20)
DIMENSION TMIN(20),IFACE(3),MISTAKE(10),MOON(15),NOON(10),W(4)
DIMENSION XC(6),XP(20),ZZ(15),CON(4),DEV(7,2),AB(3)
DIMENSION DSTANCE(20)
COMMON B, LB, OCTAL, FI, IB, T, TMIN, IFACE, MISTAKE, MOON, NOON, W, XC, XP, ZZ
COMMON CON, DEV, AB, A, NPLANE, NLINE, LMAX, MASK1, MASK2, MASK3, MASK4
COMMON ITEMP, JTEMP, MTEMP, NTEMP, IN2, IN3, IL, JA, JB, JC, JK, JL, JM, JP, JR
COMMON JT, JW, MM, KMIN, MAX, TEMP, NI, JPMAX, NIF, IX, IY, IZ, NN, MAXLAT, JJ
COMMON IP, TE, TEM, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, T1, T2
COMMON DSTANCE, FMASS, I3, TSL
COMMON MASK5, MASK6, MASK7, MASK8, MOVE, NCW
EQUIVALENCE (XP, TMIN), (LB, OCTAL)
JT=M
LDA(JT), INA(-1), ENQ(OB), DVI(NPLANE), STA(IB+3), LLS(48), ENQ(O)
DVI(NLINE), STA(IB+2), QLS(1), STQ(IB+1), ADD(IB+3), ENQ(1), STL(JT)
2340 LDA(JT), AJP(2340), RAO(IB+1)
RETURN
END

```

BOX 32

```

SUBROUTINE INVAC(MJ)
DIMENSION B(7,1500),LB(1500),OCTAL(1500),FI(3),IB(3),T(20)
DIMENSION TMIN(20),IFACE(3),MISTAKE(10),MOON(15),NOON(10),W(4)
DIMENSION XC(6),XP(20),ZZ(15),CON(4),DEV(7,2),AB(3)
DIMENSION DSTANCE(20)
COMMON B, LB, OCTAL, FI, IB, T, TMIN, IFACE, MISTAKE, MOON, NOON, W, XC, XP, ZZ
COMMON CON, DEV, AB, A, NPLANE, NLINE, LMAX, MASK1, MASK2, MASK3, MASK4
COMMON ITEMP, JTEMP, MTEMP, NTEMP, IN2, IN3, IL, JA, JB, JC, JK, JL, JM, JP, JR
COMMON JT, JW, MM, KMIN, MAX, TEMP, NI, JPMAX, NIF, IX, IY, IZ, NN, MAXLAT, JJ
COMMON IP, TE, TEM, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, T1, T2
COMMON DSTANCE, FMASS, I3, TSL
COMMON MASK5, MASK6, MASK7, MASK8, MOVE, NCW
EQUIVALENCE (XP, TMIN), (LB, OCTAL)
2360 IN2=0
MM=MJ
LIL1(MM), LDA1(LB), SCL(MASK2), SCL(MASK6), SST(MASK7), STA1(LB)
2361 NIF=0
LDA(MISTAKE+2), STA(MISTAKE+10)
DO 2370 I=1,3
IFACE(I)=0
IF(AB(I)-A-B(I,MM)) 2375,2375,2365
2375 ENA1(OB), ALS(1), STA1(IFACE), RAO(NIF), SLJ(2370)
2365 IF(B(I,MM)-A) 2380,2370,2370
2380 ENA1(OB), ALS(1), INA(-1), STA1(IFACE), RAO(NIF)
2370 CONTINUE
DO 2387 I=1,3
IB(I)=B(I,MM)/A
TEMP=IB(I)
IF(B(I,MM)/A-TEMP-0.5) 2387,2386,2386
2386 RAO1(IB)
2387 CONTINUE

```

BOX 33

```

IL=IB(3)*NPLANE+IB(2)*NLINE+IB(1)/2+1
LDA(1B+1),ADD(1B+2),ADD(1P+3),ENQ(1),STL(ITEMP),LDA(ITEMP)
AJP1(2410),STQ(JM),SLJ(2415)
2410 JM=0
2415 LDA(1B+2),ADD(1B+3),ENQ(1),STL(JL),RSC(JL),LCA(JM),ADD(JL)
+AJP3(L+3),LDA(IL),STA(NCW),LDA(MOVE),AJP1(2741),SLJ(2432),RAC(IL)
2432 JA=C
DO 2115 I=1,3
LDA1(IFACE),AJP(2115),AJP3(2115),RAO(JA),INA(-1),STA(JW)
AJP1(2120),LDA1(IFACE),STA(JB),ENA(1),STA(JD)
2115 CONTINUE
LDA(JA),AJP(2125),SLJ(2140)
2120 RAO(MISTAKE+2),SLJ(214C)
2125 ENA(0),STA(JB),STA(JD),LCA(JM),STA(JC),SLJ(2141)
2140 JC=1
2141 ENA(1),STA(JK),LDA(JM),MUI(6B),MUI(JD),INA(1),ADD(JB),ADC(JC)
STA(JW),INA(-2),AJP(2447),AJP2(2448),ENA(6),STA(JPMAX),SLJ(2700)
2447 ENA(15B),STA(JPMAX),SLJ(2700)
2448 LDA(JW),INA(-11B),AJP3(2449),ENA(11B),STA(JPMAX),SLJ(2700)
2449 ENA(5),STA(JPMAX)
2700 DO 2698 I=1,10
2698 NOON(I)=0
DO 2699 I=1,15
2699 MOON(I)=0

```

BOX 34

```

ENI1(1)
DO 2475 JP=1,JPMAX
GO TO (2701,2702,2703,2704,2705,2706,2707,2708,2709,2710,2711,
1 2712,2713,2714),JW
2701 GO TO (2455,2451,2452,2453,2454,2465),JP
2702 GO TO (2455,2451,2470,2456,2452,2453,2457,2458,2459,2454,2460,
1 2461,2462),JP
C2500 THIS SECTION IS USED WHEN THE PARTICLE SLCWS DOWN WITHIN ONE UNIT
C OF AN EDGE. WE CAN NOT CONSIDER ALL THE NEAREST NEIGHBORS IN A
C CASE LIKE THIS, ONLY CERTAIN SELECTED ONES, DEPENDING ON WHICH
C FACE IT IS THAT WE ARE NEAR.
2703 GO TO (2455,2451,2452,2453,2454),JP
2704 GO TO (2451,2452,2453,2454,2465),JP
2705 GO TO (2455,2451,2453,2454,2465),JP
2706 GO TO (2455,2452,2453,2454,2465),JP
2707 GO TO (2455,2451,2452,2453,2465),JP
2708 GO TO (2455,2451,2452,2453,2465),JP
2709 GO TO (2455,2470,2456,2457,2458,2459,2460,2461,2462),JP
2710 GO TO (2455,2451,2452,2453,2454,2458,2459,2461,2462),JP
2711 GO TO (2455,2451,2470,2453,2457,2458,2454,2460,2461),JP
2712 GO TO (2455,2452,2453,2454,2456,2457,2459,2460,2462),JP
2713 GO TO (2455,2451,2452,2453,2456,2457,2458,2459,2470),JP
2714 GO TO (2455,2451,2470,2456,2452,2454,2460,2461,2462),JP
2451 LDA(JL),ADD(NLINE),ADD(IL),SLJ(2435)
2452 LDA(IL),SUB(NLINE),ADD(JL),SLJ(2435)
2453 LDA(IL),ADD(NPLANE),ADD(JL),SLJ(2435)
2454 LDA(IL),SUB(NPLANE),ADD(JL),SLJ(2435)
2455 LDA(IL),SLJ(2435)
2456 LDA(IL),SUB(NLINE),INA(1B),ADD(JL),SLJ(2435)
2457 LDA(IL),ADD(NPLANE),INA(1B),ADC(JL),SLJ(2435)
2458 LDA(IL),ADD(NPLANE),ADD(NLINE),SLJ(2435)
2459 LDA(IL),ADD(NPLANE),SUB(NLINE),SLJ(2435)
2460 LDA(IL),SUB(NPLANE),INA(1B),ADC(JL),SLJ(2435)
2461 LDA(IL),SUB(NPLANE),ADC(NLINE),SLJ(2435)
2462 LDA(IL),SUB(NPLANE),SUB(NLINE),SLJ(2435)
2465 LDA(IL),INA(-1),SLJ(2435)
2470 LDA(IL),ADD(NLINE),ADD(JL),INA(1)
2435 STA(ITEMP),AJP(2475),AJP3(2475),SUB(MAXLAT),+AJP(L+1),AJP2(2475)
LDA(ITEMP),STA(MOON),INI1(1)
2475 CONTINUE

```

BOX 35

```

INI1(-1),SIL1(JPMAX),LDA(MOVE),AJP1(2741)
2480 ENA(1),STA(JP)
DO 2485 K=1,JPMAX
LDA3(MOON),STA(ITEMP),LIL1(ITEMP),LDQ1(LB),LDL(4B),AJP1(2485)
2485 ENQ1(0),LIL1(JP),STQ1(NOCN),RAO(JP)
CONTINUE
LDA(JP),INA(-1),STA(JK)

```

BOX 36

```

LDA(JK),INA(-1),AJP(2490),AJP2(2510),LCA(IN2),AJP1(2720),SLJ(2600)
2490 LDA(NOON+1),STA(IL)
2492 CALL SITE(IL)
2493 DO 2495 I=1,3
TEMP=IB(I)
B(I,MM)=A*TEMP
2495 CONTINUE
ENA(3),STA(NI),LIL1(IL),LIL3(MM),LDA(IL),ALS(27),STA(ITEMP)
LDA3(LB),LDQ(MASK2),SSU(ITEMP),STA3(LB),LDA1(LB),SST(4B),STA1(LB)
LDA(IN2),AJP1(2800)
RETURN

```

BOX 37

```

2510 DO 2512 K=1,JK
LDA3(NOON),STA(ITEMP),LDA(C.O),STA3(DSTANCE)
CALL SITE(ITEMP)
DO 2512 I=1,3
TEMP=IB(I)
TEMP=TEMP*A
2512 DSTANCE(K)=DSTANCE(K)+(TEMP-B(I,MM))*(TEMP-B(I,MM))
ENI2(1)
DO 2514 K=1,JK
LDA3(DSTANCE),FSB2(DSTANCE),AJP(2514),AJP2(2514),SIL3(ITEMP)
LIL2(ITEMP)
2514 CONTINUE
ENI5(1),LDA2(NOON),STA5(MOCN),INI5(1)
DO 2516 K=1,JK
LDA2(DSTANCE),FSB3(DSTANCE),+AJP(L+1),AJP2(2516),+SIL2(ITEMP)
LAC(ITEMP),INA3(0),AJP(2516),LDA3(NOCN),STA5(MOON),INI5(1)
2516 CONTINUE
INI5(-1),ENA5(0),INA(-1),AJP1(L+3),+LDA2(NOON),STA(IL),+SLJ(2492)
+ENA5(0),STA(MMAX)
DO 2518 K=1,MMAX
LDA(MM),SUB3(MOON),AJP(2520)
2518 CONTINUE
2520 ENA3(0),AJP(L+3),LDA3(MOCN),STA(IL),+SLJ(2492),+ENQ6(0),LCL(MASK5)
+AJP1(L+2),LDA(MOON+2),STA(IL),SLJ(2492),+LDA(MOCN+1),STA(IL)
SLJ(2492)

```

BCX 38

```

2600 T1=0.0
      DO 2605 I=4,6
2605 T1=T1+B(I,MM)*B(I,MM)
      ENA(1),STA(JA),LDA(T1),AJP1(2620),ENA(0),STA(JA),SLJ(2620)
2620 T2=0.0
      DO 2645 K=1,JPMAX
      LDA3(MOON),STA(ITEMP),ALS(27),STA(JTEMP)
      DO 1700 I=1,LMAX
      LDQ1(LB),LDL(MASK2),SUB(JTEMP),AJP1(1700),LDL(MASK1),AJP(2621)
      LDA(TSL),FMU(1.0E+3),STA3(TMIN),SLJ(2645)
1700 CONTINUE
2621 CALL SITE(ITEMP)
      DO 2625 I=1,3
      TEMP=IB(I)
2625 FI(I)=A*TEMP
      LDA(JA),AJP1(2635)
      DO 2630 I=1,3
2630 TMIN(K)=TMIN(K)+(B(I,MM)-FI(I))*(B(I,MM)-FI(I))
      GO TO 2645
2635 DO 2640 I=1,3
2640 T2=T2+(B(I,MM)-FI(I))*B(I+3,MM)
      TMIN(K)=-T2/T1
2645 CONTINUE
      ENA(1),STA(KMIN),LDA(JPMAX),INA(-1),STA(JK)
      DO 2660 K=1,JK
      IF(TMIN(K)-TMIN(K+1))266C,2660,2650
2650 IF(TMIN(K+1)-TMIN(KMIN)) 2655,2660,266C
2655 KMIN=K+1
2660 CONTINUE
      LIL1(KMIN),LDA1(MOON),STA(IP),LDA(TSL),FMU(100.0),STA(TEM)
      LDA1(TMIN),+FSB(TEM),AJP3(L+2),ENI1(0),SLJ(2685)
      CALL SITE(IP)
      DO 2665 I=1,3
      TEMP=IB(I)
      FI(I)=A*TEMP
2665 T(I)=ABSF(B(I,MM)-FI(I))
      LDA(JB),INA(1),ARS(1),STA(ITEMP),LIL1(ITEMP),LDA(C.0),STA1(T)
      ENA(1),STA(MAX)
      DO 2675 I=1,2
      LDA1(T),FSB1(T+1),AJP(2675),AJP2(2675),SIL1(MAX),RAO(MAX)
2675 CONTINUE
      DO 2680 I=1,LMAX
      LDQ1(LB),LDL(MASK2),ARS(27),SUB(IP),AJP(2685)
2680 CONTINUE
2686 STA(MM),ENA(1),STA(IN2),SLJ(2361)

```

BOX 39

```

2800 LDA(IP),STA(IL),LDA(MJ),STA(MM),ENA(C),STA(IN2),SLJ(2492)
THIS IS THE SECTION OF INVAC THAT MAKES THE INTERSTITIALS. THE REST OF
THE SUBROUTINE IS CONCERNED ONLY WITH VACANCIES
2720 TEMP=B(MAX,MM)-B(MAX,MJ)
CALL SITE (IP)
DO 2725 I=1,3
T2=IB(I)
B(I,MM)=A*T2
2725 B(I,MJ)=B(I,MM)
IF(TEMP) 2735,2730,2730
2730 B(MAX,MM)=B(MAX,MM)+0.5*A
B(MAX,MJ)=B(MAX,MJ)-0.5*A
GO TO 2740
2735 B(MAX,MM)=B(MAX,MM)-0.5*A
B(MAX,MJ)=B(MAX,MJ)+0.5*A
2740 CONTINUE
LDA(IP),ALS(27),STA(ITEMP),LDA(MM),ALS(15),ADD(ITEMP),STA(JA)
LDQ(MASK3),LIL3(MJ),LDA3(LB),SSU(JA),STA3(LB),ENA3(O),ALS(15)
ADD(ITEMP),STA(JA),LIL1(MM),LDA1(LB),SSU(JA),STA1(LB),LIL1(IP)
LDA1(LB),SST(4B),STA1(LB),LDA(MM),SUB(MJ),AJPI(2741)
RAO(MISTAKE+4)
2741 RETURN
END

```

BOX 40

```

SUBROUTINE INTER(MQ,II,S)
DIMENSION B(7,1500),LB(1500),OCTAL(1500),FI(3),IB(3),T(20)
DIMENSION TMIN(20),IFACE(3),MISTAKE(10),MOON(15),NOON(10),W(4)
DIMENSION XC(6),XP(20),ZZ(15),CCN(4),DEV(7,2),AB(3)
DIMENSION DSTANCE(20)
COMMON B, LB, OCTAL, FI, IR, T, TMIN, IFACE, MISTAKE, MOON, NOON, W, XC, XP, ZZ
COMMON CON, DEV, AB, A, NPLANE, NLINE, LMAX, MASK1, MASK2, MASK3, MASK4
COMMON ITEM, JTEMP, MTEMP, NTEMP, IN2, IN3, IL, JA, JB, JC, JK, JL, JM, JP, JR
COMMON JT, JW, MM, KMIN, MAX, TEMP, NI, JPMAX, NIF, IX, IY, IZ, NN, MAXLAT, JJ
COMMON IP, TE, TEM, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, T1, T2
COMMON DSTANCE, FMASS, I3, TSL
COMMON MASK5, MASK6, MASK7, MASK8, MOVE, NOW
EQUIVALENCE (XP, TMIN), (LB, CCTAL)
MM=MQ
DO 1C I=1,6
XP(I)=B(I,MM)-B(I,II)
FMU(0.5) STA(ZZ+2) .
10 XC(I)=ZZ(2)
ZZ(9)=(XP(4)*XP(4)+XP(5)*XP(5)+XP(6)*XP(6))*1.0E8
FMU(C4) STA(ZZ+10).
ZZ(1)=SQRTF(ABSF(ZZ(9)))
ZZ(10)=1.0/ZZ(10)
ZZ(11)=S*S
ZZ(7)=C1

```

BOX 41

```

15 ZZ(2)=C2/EXPF(ZZ(7)*C3)
   FSB(C9)                      FMU(ZZ+10).
   STA(ZZ+8)
   ZZ(2)=C3*ZZ(2)*ZZ(7)*ZZ(10)*ZZ(7)
   ZZ(5)=ZZ(7)*(1.0-ZZ(8))
   ZZ(2)=ZZ(7)-(ZZ(7)*ZZ(5)-ZZ(11))/(2.0*ZZ(5)+ZZ(2))
   LDA(ZZ+2)
   FSB(ZZ+7)  AJP2(19)
   LDA(ZZ+2)
   FMU(1.000001)                FSB(ZZ+7) .
   AJP2(20)                      LDA(ZZ+2) .
   STA(ZZ+7)                      SLJ(15) .
19 ZZ(2)=ZZ(7)

```

BOX 42

```

20 LDA(0.0)                      STA(ZZ+5) .
   STA(ZZ+6)                      LDA(ZZ+2) .
   FMU(ZZ+2)                      STA(ZZ+7) .
   ZZ(8)=C2/EXPF(ZZ(2)*C3)-C9
   LAC(ZZ+2)                      FMU(C8) .
   FAD(1.0)                      STA(ZZ+4) .
   DO 25 I=1,4
   ZZ(9)=ZZ(4)*CON(I)
   ZZ(3)=ZZ(2)*ZZ(2)
   ZZ(15)=ZZ(3)*ZZ(10)/ZZ(9)
   ZZ(14)=ZZ(11)*(2.0-ZZ(9))
   ZZ(9)=1.0-ZZ(9)
   ZZ(12)=1.0/ZZ(9)
   ZZ(9)=C2/EXPF(ZZ(2)*ZZ(12)*C3)-C9
   ZZ(9)=W(I)/SQRTF(ABSF(ZZ(14)+ZZ(15)*(ZZ(8)-ZZ(9))))
   FAD(ZZ+5)                      STA(ZZ+5) .
   LDA(ZZ+9)                      FMU(ZZ+12) .
   FMU(ZZ+12)                    FAD(ZZ+6) .
   STA(ZZ+6)                      .
25 CONTINUE
   ZZ(7)=2.0*SQRTF(ABSF(ZZ(4)))
   ZZ(5)=S*ZZ(5)*ZZ(7)
   ZZ(6)=ZZ(3)*ZZ(6)*ZZ(7)/ZZ(1)

```

BOX 43

```

ZZ(7)=SINF(ZZ(5))*C6
ZZ(8)=COSF(ZZ(5))
ZZ(3)=ZZ(5)+ZZ(13)
ZZ(4)=SINF(ZZ(3))*ZZ(1)*C.5E-4
ZZ(10)=C5*ZZ(1)*COSF(ZZ(3))

```

BOX 44

```

FI(1)=XP(2)*XP(6)-XP(3)*XP(5)
FI(2)=XP(3)*XP(4)-XP(1)*XP(6)
FI(3)=XP(1)*XP(5)-XP(2)*XP(4)
ZZ(1)=FI(2)*XP(3)-FI(3)*XP(2)
ZZ(2)=FI(3)*XP(1)-FI(1)*XP(3)
ZZ(3)=FI(1)*XP(2)-FI(2)*XP(1)
FMU(ZZ+3)          STA(TEMP) .
LDA(ZZ+2)          FMU(ZZ+2) .
FAD(TEMP)          STA(TEMP) .
LDA(ZZ+1)          FMU(ZZ+1) .
FAD(TEMP)          STA(TEMP) .
TEMP=SQRTF(ABSF(TEMP))
LDA(1.0)           FDV(TEMP) .
STA(TEMP)          LDA(ZZ+1) .
FMU(TEMP)          STA(ZZ+1) .
LDA(ZZ+2)          FMU(TEMP) .
STA(ZZ+2)          LDA(ZZ+3) .
FMU(TEMP)          STA(ZZ+3) .

```

BOX 45

```

DO 30 I= 1,3
I3=I+3
ZZ(5)=XC(I)*ZZ(8)+ZZ(I)*ZZ(7)
ZZ(9)=B(I,I1)+XC(I)+(B(I3,I1)+XC(I3))*ZZ(6)*1.0E14
DEV(I,1)=ZZ(9)+ZZ(5)
DEV(I,2)=ZZ(9)-ZZ(5)
ZZ(5)=XC(I)*ZZ(10)+ZZ(I)*ZZ(4)
ZZ(9)=B(I3,I1)+XC(I3)
DEV(I3,1)=ZZ(9)+ZZ(5)
30 DEV(I3,2)=ZZ(9)-ZZ(5)
LDA(0.0),STA(T1),STA(T2)
DO 29 I=4,6
T1=T1+DEV(I,1)*DEV(I,1)
29 T2=T2+DEV(I,2)*DEV(I,2)
DEV(7,1)=FMASS*T1*0.5180C761500
DEV(7,2)=FMASS*T2*0.5180C761500
END

```

BOX 1

```

PROGRAM SLAVE
DIMENSION AB(3),B(7,2370),FI(3),IB(3),LB(2370),XYZ(3),EMAX(30)
DIMENSION YENTRY(10),ZENTRY(10),CCTAL(2370),KET(26)
DIMENSION IHISTO(105),NUMBERS(50),MISTAKE(10)
DIMENSION NSIDE(6),ESIDE(6),NITEMP(10),IC(100),TSLI(30),NTSC(30)
COMMON IX,IY,IZ,FI,A,NLINE,NPLANE,LMAX,IB,LB,XYZ,MAXLAT,B,OCTAL
COMMON IHISTO,NUMBERS,AB,IL,ITEMP,ITEM,IT,TEMP,TEM,KET
COMMON NSUBST,EBUL,ETHERM,NSIDE,NBUL,NSAME,INTERST,INPAIRS,NFACE
COMMON ESIDE,NVAC,ECAL,OENERGY,NITEMP,DEPTH,PERDIST,IC,EPB
COMMON YENTRY,ZENTRY
EQUIVALENCE(LB,OCTAL)
REWIND 8
PRINT 109
READ TAPE 8, IX,IY,IZ,AB,NLINE,NPLANE,MAXLAT,LMAX,A,SPHI,FMASS,
1 ETHRESH,THERMAL,EPB,LULL,ALPHA,BETA,NTS,MNTS,TTIME,TSLI,NTSC,
2 OENERGY,TENERGY,MISTAKE, YENTRY,ZENTRY,NA,EMAX,EFOUND
READ TAPE 8,(LB(L),(B(I,L) I=1,7) L=1,LMAX)
WRITE OUTPUT TAPE 3,398
398 FORMAT(30H SET SLJ SWITCH 2 UP IF NEEDED)
SLS(399)
399 CONTINUE
PRINT 101
DO 400 I=1,6
READ INPUT TAPE 2,100
100 FORMAT(80H
)
400 PRINT 100
READ INPUT TAPE 2,405,(KET(I) I=1,25)
405 FORMAT(10X,13I4)
KET(26)=1000
SLJ2(200) SLJ(220)
200 PRINT 210
210 FORMAT(40H SELECTIVE JUMP SWITCH NUMBER TWO WAS UP)
220 PRINT 101
101 FORMAT(////)
IHISTO(1)=5H(I3,F
IHISTO(2)=4H7.1,
IHISTO(3)=5H3H P.
IHISTO(4)=6H4HC.
IHISTO(105)=1H)
ITEMP=32768
I2E15=ITEMP
I2E24=ITEMP*512
F2E24=I2E24
I2E30=ITEMP*ITEMP
MASK25=77770B
MASK69=7777000000B
MASK13=77770000000000B
MASK14=70000000000000B
MASKSA=100000000000000B
MASKSU=200000000000000B
MASKSET=73000000000000007B

```

BOX 2

```
+LDA(NTS) AJP1(L+2) LDA(MNTS) STA(NTS)
NSUBST=0
EBUL=0.0
ETHERM=EFOUND
DO 1405 I=1,6
1405 ESIDE(I)=0.0
NSIDE(I)=0
NBUL=0
NSAME=0
INTERST=0
NAA=NA-1
DO 1407 I=1,NAA
1407 TSLI(I)=TSLI(I)*1.0E-14
TTIME=TTIME*1.0E-14
DO 1410 L=1,LMAX
+LDA4(LB) SCL(MASKSET) SLJ2(L+2) SCL(MASK69) SCL(MASK13) +STA4(LB)
1410 CONTINUE
```

BOX 3

```

1411 DO 1449 L=1,LMAX
      LDQ4(LB) LDL(MASK14)
      AJP(1415) ALS(9)
      STA(NFACE)
1412 NSIDE(NFACE)=NSIDE(NFACE)+1
      ESIDE(NFACE)=ESIDE(NFACE)+B(7,L)
      GO TO 1449
1415 SLJ2(1416)
      CALL ROUND(L)
      +SLJ(L+3)
1416 +LDQ4(LB) LDL(MASK13) ARS(27) STA(IL)
      LIL1(IL) LDA(IL) ALS(27) STA(IL27)
      SLJ2(1417) LDA4(LB) SST(IL27) STA4(LB)
1417 TEMP=B(7,L)-THERMAL
      AJP3(1425) RAC(NBUL)
      EBUL=EBUL+B(7,L)
      LCA4(LB) SST(28) STA4(LB)
      TEM=B(7,L)-ETHRESH
      AJP2(1449)
      CALL ROUND(L)
      LIL1(IL)
      LDA1(LB) SST(48) STA1(LB)
      GO TO 1449
1425 ETHERM=ETHERM+B(7,L)
      SLJ2(1445) LDC1(LB)
      LDL(48) AJP(1427)
      DO 1426 J=1,L
      LDQ2(LB) LDL(MASK13)
      SUB(IL27) AJP1(1426)
      LDQ2(LB) LDL(28)
      AJP1(1426)
      ITEMP=L
      ALS(15) ADD2(LB) SCL(MASKSA) SCL(MASKSU) STA2(LB)
      ITEMP=J
      ALS(15) ADD4(LB) SCL(MASKSA) SCL(MASKSU) STA4(LB)
      SLJ(1444)
1426 CONTINUE
1427 LDA1(LB) SST(48) STA1(LB)
      LAC(IL) INA4(C) AJP(1428) LCA(MASKSU)
      ADD4(LB) STA4(LB) SLJ(1444)
1428 LDA(MASKSA) ADD4(LB) STA4(LB)
1444 LDA1(LB) SST(48) STA1(LB) SLJ(1449)
1445 LDA1(LB) SST(48) STA1(LB)
      +LDQ4(LB) LDL(MASK13) ARS(27) STA(IL)
      +LIL1(IL) LDA1(LB) SST(18) STA1(LB)
      +LDL(MASK69) AJP1(1449) LAC(IL) INA4(O)
      +AJP1(L+3) LCA4(LB) SST(MASKSA) STA4(LB) .SLJ(1449)
      +LDA4(LB) SST(MASKSU) STA4(LB)
1449 CONTINUE
      NVAC=0
      DO 1456 L=1,LMAX
      LDQ4(LB) LDL(48) AJP1(1450) RAO(NVAC)
1450 LDQ4(LB) LDL(MASKSA) AJP(1451) RAO(NSAME)
1451 LDQ4(LB) LDL(MASKSU) AJP(1452) RAC(NSUBST)
1452 LDQ4(LB) LDL(MASK69) AJP(1456) RAO(INTERST)
      NVAC=NVAC+MAXLAT-LMAX

```

BCX 4

```
TEMP=ESIDE(1)
ITEMP=NSIDE(1)
DO 1457 I=2,6
ITEMP=ITEMP+NSIDE(I)
1457 TEMP=TEMP+ESIDE(I)
ECAL=ETHERM+EBUL+TEMP
LMAXCAL=INTERST+NSAME+NSLBST+NBUL+ITEMP
PRINT 1458,IX,AB(1),IY,AB(2),IZ,AB(3),MAXLAT,A,SPHI,FMASS,ETRESH,
1THERMAL
1458 FORMAT( 29H THE LATTICE DIMENSIONS ARE -5X,11HX-DIRECTIONI6, 6H
1 X A =F8.3, 10H ANGSTROMS/34X, 11HY-DIRECTIONI6,6H X A =F8.3, 10H
2 ANGSTROMS/34X, 11HZ-DIRECTIONI6,6H X A =F8.3, 10H ANGSTROMS// 21H
3 THE LATTICE CONTAINS I5,6H ATOMS//33H THE LATTICE SPACING CONSTANT
4 A =F6.3, 10H ANGSTROMS/27H THE SPHERE OF INFLUENCE ISF12.3, 10H
5 ANGSTROMS/ 19H THE ATOMIC MASS ISF20.3,4H AMU//
6 40H THRESHOLD ENERGY FOR VACANCY PRODUCTIONF8.3,4H EV./
7 25H THERMAL THRESHOLD ENERGYF23.3,4H EV.)
LDA(ALPHA) FMU(180.0) FCV(3.1415926536) STA(YANGLE)
LDA(BETA) FMU(180.0) FCV(3.1415926536) STA(ZANGLE)
IT=LMAX-MAXLAT
PRINT 101
PRINT 1454,IT,LULL,EPB,ALPHA,YANGLE,BETA,ZANGLE
1454 FORMAT(23H CONDITIONS OF THIS RUN///I3, 20H ATOMS WERE SHOT IN.
128H ONE ATOM WAS SHOT IN EACHI3,11H TIME STEPS/
3 38H ORIGINAL ENERGY OF EACH INCOMING ATOMF12.3,4H EV.///
4 28H DIRECTION OF INCOMING ATOMS/
526H ALPHA = ARCTAN( VY/VX ) =F8.4,11H RADIANS =F8.3,8H DEGREES/
626H BETA = ARCTAN( VZ/VX ) =F8.4,11H RADIANS =F8.3,8H DEGREES)
ITEMP=MAXLAT+1
PRINT 1453,(L,YENTRY(L-MAXLAT),ZENTRY(L-MAXLAT) L=ITEMP,LMAX)
1453 FORMAT(///37H POSITIONS OF ENTRY OF INCOMING ATOMS//7H NUMBER,9X,
11HX9X,1HY9X,1HZ//(I6,8X,5HO.COC,2F10.3))
PRINT 1455,NTS,MNTS,ITIME,ITSLI(I),NTSC(I) I=1,NA)
1455 FORMAT(1H1,// 41H THE NUMBER OF TIME STEPS OF THIS RUN WASI10/
1 47H THE LIMIT SET FOR THE NUMBER OF TIME STEPS WASI4/ 31H THE
2TOTAL TIME OF THIS RUN WASIPE12.5,8H SECONDS// 41H TIME STEP LENGT
3H NUMBER OF FIRST TIME/4X, 36HIN SECCNDS STEP OF THIS L
4LENGTH/(/1PE14.4,I18))
LDA(NTS) SUB(30) +AJP2(L+2) LDA(NTS) STA(IT) SLJ(5541)
LDA(30) STA(IT)
5541 CONTINUE
```

```

PRINT 1459,ECAL,TENERGY,CENERGY,ETHERM,(I,EMAX(I) I=1,IT)
1459 FORMAT(1H1,728H THE ENERGY ACCOUNTED FOR IS F14.3,4H EV./
1 28H SUM OF ENERGIES OF ATOMS F14.3,4H EV./
2 28H ENERGY SHOT INTO LATTICE F14.3,4H EV./
3 45H ENERGY ABSORBED BY LATTICE AS THERMAL ENERGY F12.3,4H EV.//
4 29H NUMBER OF ENERGY OF MOST/
5 29H TIME STEP ENERGETIC ATOM// (I7,F16.3,3H EV))
INTERST=INTERST/2
PRINT 1460,LMAXCAL,LMAX,NSAME,NSUBST,INTERST,NVAC
1460 FORMAT(1H1,738H THE NUMBER OF ATOMS ACCOUNTED FOR IS I5/
1 38H THE TOTAL NUMBER OF ATOMS IS I5//
2 38H THE NUMBER IN ORIGINAL POSITIONS IS I5//
3 38H THE NUMBER OF REPLACEMENTS IS I5//
4 38H THE NUMBER OF INTERSTITIAL PAIRS IS I5//
5 38H THE NUMBER OF VACANT LATTICE SITES IS I5/////))
IF(MISTAKE(1)) 9955,9955,9956
9955 PRINT 9957
9957 FORMAT(30H THE ENERGY CHECK DID NOT FAIL )
GO TO 9965
9956 PRINT 9959,MISTAKE(1)
9959 FORMAT(24H THE ENERGY CHECK FAILED I4,16H DIFFERENT TIMES)
9965 IF(MISTAKE(2)) 9961,9961,9962
9961 PRINT 9963
9963 FORMAT(62H NO INTERSTITIALS OR VACANCIES OCCURED ALONG AN EDGE OR
1 CORNER )
GO TO 9966
9962 PRINT 9960,MISTAKE(2)
9960 FORMAT(60H AN INTERSTITIAL OR VACANCY OCCURRED ALONG AN EDGE OR CO
1 RNER I4,16H DIFFERENT TIMES)
9966 CONTINUE
PRINT 101
PRINT 1462
1462 FORMAT(24X,6HNUMBER,5X,12HTOTAL ENERGY/5H FACE,6X,5HGROUP,7X,
18HIN GROUP,7X,6HIN EV.//)
PRINT 1464,NBUL,EBUL,(NSIDE(I),ESIDE(I) I=1,6)
1464 FORMAT(19H KNOCK-ONS I9,F16.3/19H 1 FRONT FACE IS,F16
1.3/19H 2 BACK FACE I9,F16.3/19H 3 LEFT FACE I9,F16.3/
2 19H 4 RIGHT FACE I9,F16.3/19H 5 TOP FACE I9,F16.3/
3 20H 6 BOTTOM FACE I8,F16.3)

```

BOX 5

```

1465 PRINT 1465, NSAME
1465 FORMAT(1H1, 1X, 59H THE NUMBER OF ATOMS THAT ARE IN THEIR INITIAL PO
1 SITICNS ISI5//10H THEY ARE/)
ITEM=77777770000777778
IT=7770000777777778
J=1
K=1
L=1
DO 1466 I=1, 10
1466 NUMBERS(I)=0
DO 1480 M=1, LMAX
IF(J-11) 1474, 1467, 1467
1467 PRINT 1472, (NUMBERS(I) I=1, 10)
DO 1468 I=1, 10
1468 NUMBERS(I)=0
J=1
L=L+1
IF(K-501) 1470, 1469, 1469
1469 PRINT 109
K=1
L=1
GO TO 1474
1470 IF(L-11) 1474, 1471, 1471
1471 PRINT 110
L=1
1472 FORMAT(10I10)
1474 LDA5(LB) SCL(IT) ARS(27) STA(ITEMP)
LAC(ITEMP) INAS(0) AJP1(1476) LDA5(LB)
SCL(ITEM) AJP1(1476)
NUMBERS(J)=M
1476 J=J+1
1480 K=K+1
INI2(-1) SIL2(IT) LDA(IT) AJP(480)
480 PRINT 1472, (NUMBERS(I) I=1, IT)

```

BOX 6

```

1560 PRINT 1560, NVAC
1560 FORMAT(1H1, 1X, 37H THE NUMBER OF VACANT LATTICE SITES ISI6///10H THE
1 Y ARE //)
IT=1
DO 1565 L=1, MAXLAT
1562 LDQ4(LB) LDL(4B) AJP1(1565)
NUMBERS(IT)=L
RAO(IT) SUB(51) AJP1(1565)
PRINT 1472, (NUMBERS(IT) IT=1, 50)
IT=1
1565 CONTINUE
1566 PRINT 1472, (NUMBERS(I) I=1, IT)

```

BOX 7

```

PRINT 109
PRINT 1499
1499 FORMAT(13H REPLACEMENTS//)
PRINT 1500, NSUBST
1500 FORMAT(1X, 30H THE NUMBER OF REPLACEMENTS IS I6///
1 INITIAL FINAL PENETRATION PENETRATION IN/ 55H
DO 1502 I=1, 100 . 56H
1502 IC(I)=0
DO 1517 L=1, LMAX
LDQ4(LB) LDL(MASKSU) AJP(1517) LDL(MASK13) ARS(27) STA(IL)
CALL INITIAL(L)
CALL DEPTH(L)
PRINT 1515, L, IL, DEPTH, PERDIST
1515 FORMAT(17, I10, F16.3, F18.3)
1517 CONTINUE
1518 PRINT 109
PRINT 1499
PRINT 1520
1520 FORMAT(40H DISTRIBUTION OF X-DIRECTION PENETRATION//21X,
117HR A N G E18X, 6HNUMBER/)
DO 1521 I=1, 30
J=I-7
TEM=J
TEM=TEM-0.5
TEMP=TEM+1.0
1521 PRINT 1525, J, TEM, TEMP, IC(I)
1525 FORMAT(13, F11.1, 9H X A - 16HX PENETRATION -F6.1, 4H X A111)
DO 1527 I=1, 30
1527 NUMBERS(I)=IC(I)
IL=-7
CALL HISTO(30)
PRINT 109
PRINT 1499
PRINT 1530
1530 FORMAT(35H DISTRIBUTION OF RADIAL PENETRATION//21X,
117HR A N G E22X, 6HNUMBER/)
DO 1531 I=1, 20
IT=I-1
1531 PRINT 1532, I, IT, I, IC(I+30)
1532 FORMAT(13, I9, 9H X A - 21HRADIAL PENETRATION -I4, 4H X A112)
DO 1533 I=1, 20
1533 NUMBERS(I)=IC(I+30)
CALL HISTO(20)

```

BOX 8

```

PRINT 109
PRINT 1534
1534 FORMAT(19H INTERSTITIAL PAIRS//)
PRINT 1535,INTERST
1535 FORMAT(10H THERE ARE I4,15H INTERSTITIAL PAIRS//11H NUMBERS OF/104H
1 THE PAIR NUMBER PENETRATION OF L PENETRATION OF L
2 PENETRATION OF LL PENETRATION OF LL/ 105H
3 L LL OF SITE IN X-DIRECTION IN RADIAL DIRECTION
4 IN X-DIRECTION IN RADIAL DIRECTION//)
DO 1538 I=1,100
1538 IC(I)=0
DO 1550 L=1,LMAX
LDQ4(LB) LDL(2B) AJP1(1550)
LDQ4(LB) LDL(MASK69) AJP(1550) ARS(15)
STA(LL) LDL(MASK13) ARS(27) STA(IL)
LIL1(LL) LDQ1(LB) LDL(2B) AJP1(1550)
CALL INITIAL(L)
CALL DEPTH(L)
TE =DEPTH
TEM=PERDIST
CALL INITIAL(LL)
CALL DEPTH(LL)
1545 PRINT 1545,L,LL,IL,TE,TEM,DEPTH,PERDIST
1550 FORMAT(15,I6,19,F16.4,F20.4,F22.4,F21.4)
CONTINUE
DO 1555 I=1,100
1555 IC(I)=IC(I)/2
PRINT 109
PRINT 1534
PRINT 1520
DO 1556 I=1,30
J=I-7
TEM=J
TEM=TEM-0.5
TEMP=TEM+1.0
1556 PRINT 1525,J,TEM,TEMP,IC(I)
DO 1557 I=1,30
1557 NUMBERS(I)=IC(I)
IL=-7
CALL HISTO(30)
PRINT 109
PRINT 1534
PRINT 1530
DO 1558 I=1,20
IT=I-1
1558 PRINT 1532,I,IT,I,IC(I+30)
DO 1559 I=1,20
1559 NUMBERS(I)=IC(I+30)
CALL HISTO(20)

```

BOX 9

```

LDA(NBUL)  AJP(9951)
1571 PRINT 109
PRINT 1572
1572 FORMAT(10H KNOCK-ONS//)
PRINT 573,NBUL
573 FORMAT(10H THERE ARE15,1CH KNOCK-ONS//)
PRINT 574
574 FORMAT(91X,11HPENETRATION/4H L7X,1HX8X,1HY8X,1HZ8X,2HVX7X,2HVV7X
1,2HVZ5X,6HENERGY7X,5HLB(L)1CX, 11HX RADIAL//)
1576 FORMAT(15,7F9.3,3X,015,2F8.2)
DO 1577 I=1,100
1577 IC(I)=0
IT=1
DO 1578 L=1,LMAX
LDQ4(LB) LDL(2B) AJP(157E)
LDA(IT) SUB(51) AJP1(1567)
PRINT 109
PRINT 1572
PRINT 574
IT=1
1567 CALL INITIAL(L)
CALL DEPTH(L)
CALL ECOUNT(L)
PRINT 1576,L,(B(I,L) I=1,7),OCTAL(L),DEPTH,PERDIST
RAQ(IT)
1578 CONTINUE
PRINT 109
PRINT 1572
PRINT 1520
DO 1569 I=1,30
J=I-7
TEM=J
TEM=TEM-0.5
TEMP=TEM+1.0
1569 PRINT 1525,J,TEM,TEMP,IC(I)
DO 1579 I=1,30
1579 NUMBERS(I)=IC(I)
IL=-7
CALL HISTO(30)
PRINT 109
PRINT 1572
PRINT 1530
DO 1574 I=1,20
IT=I-1
1573 NUMBERS(I)=IC(I+30)
1574 PRINT 1532,I,IT,I,IC(I+30)
IL=0
CALL HISTO(20)
PRINT 109
PRINT 1572
PRINT 1580
1580 FORMAT(23H DISTRIBUTION OF ENERGY//
115X17HR A N G E14X,6HNUMBER/)
DO 1680 I=1,25
1680 PRINT 1526,I,KET(I),KET(I+1),IC(I+50)
1526 FORMAT(13,17,21H EV - ENERGY -16,3H EV110)
DO 1681 I=1,25
1681 NUMBERS(I)=IC(I+50)
CALL HISTO(25)

```

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9951 DO 1599 J=1,6
      IF (J-1) 1581,1581,1583
1581 PRINT 1582,NSIDE(1)
1582 FORMAT(1H1,1X,16HSPUTTERED ATOMS-110,22H ATOMS WERE SPUTTERED.)
      GO TO 1585
1583 PRINT 1584,J,NSIDE(J)
1584 FORMAT(1H1,1X,45HTHE NUMBER OF ATOMS WHICH EXITED THROUGH SIDE12,3
1H ISI5)
1585 LDA2(NSIDE) AJP(1599) AJP3(1599)
      PRINT 1586
1586 FORMAT(///91X, 23HPENETRATION TIME STEP/4H L7X,1HX8X,1HY8X,1
1HZ8X,2HVX7X,2HVV7X,2HVZ5X,6HENERGY7X,5HLB(L)10X,22HX RADIAL
2OF EXIT//)
1587 FORMAT(15,7F9.3,3X,015,2F8.2,19)
      NFACE=0
      DO 1589 I=1,100
1589 IC(I)=0
      NTS=0
      DO 1595 L=1,LMAX
      LDQ4(LB) LDL(MASK14) AJP(1595) ALS(9)
      STA(NFACE) SIL2(IT) SUB(IT) AJP1(1595)
      LDL(MASK25) ARS(3) STA(NTS)
1594 CALL INITIAL(L)
      CALL DEPTH(L)
      CALL ECOUNT(L)
      PRINT 1587,L,(B(I,L) I=1,7),OCTAL(L),DEPTH,PERDIST,NTS
1595 CONTINUE
      PRINT 1695,J
1695 FORMAT(1H1,12H EXITED FACEI4//)
      PRINT 1520
      DO 1696 I=1,30
      L=I-7
      TEM=L
      TEM=TEM-0.5
      TEMP=TEM+1.0
1596 NUMBERS(I)=IC(I)
1696 PRINT 1525,L,TEM,TEMP,IC(I)
      IL=-7
      CALL HISTO(30)
      PRINT 1695,J
      PRINT 1530
      DO 1697 I=1,20
      IT=I-1
1597 NUMBERS(I)=IC(I+30)
1697 PRINT 1532,I,IT,I,IC(I+30)
      IL=0
      CALL HISTO(20)
      PRINT 1695,J
      PRINT 1580
      DO 1698 I=1,25
1598 NUMBERS(I)=IC(I+50)
1698 PRINT 1526,I,KET(I),KET(I+1),IC(I+50)
      CALL HISTO(25)
1599 CONTINUE

```

BOX 11

```

SLJ1(120)
PRINT 119
107 L=1
108 PRINT 118,L,(B(I,L) I=1,7),OCTAL(L)
109 FORMAT(1H1)
110 FORMAT(/)
111 DO 117 L=2,LMAX
112 IF(10*((L-1)/10)-L+1) 117,113,113
113 IF(50*((L-1)/50)-L+1) 116,114,114
114 PRINT 119
115 GO TO 117
116 PRINT 110
117 PRINT 118,L,(B(I,L) I=1,7),OCTAL(L)
118 FORMAT(15,7F9.3,3X,015)
119 FORMAT(1H1,///13H LATTICE DUMP///4H L7X,1HX8X,1HY8X,1HZ8X,2HVX7X
1,2HVY7X,2HVZ5X,6HENERGY 7X,5HLB(L)//)
120 END

```

BOX 12

```

SUBROUTINE ROUND(L)
DIMENSION AB(3),B(7,2370),FI(3),IB(3),LB(2370),XYZ(3),EMAX(30)
DIMENSION YENTRY(10),ZENTRY(10),OCTAL(2370),KET(26)
DIMENSION IHISTO(105),NUMBERS(50),MISTAKE(10)
DIMENSION NSIDE(6),ESIDE(6),NITEMP(10),IC(100),TSLI(30),NTSC(30)
COMMON IX,IY,IZ,FI,A,NLINE,NPLANE,LMAX,IB,LB,XYZ,MAXLAT,B,OCTAL
COMMON IHISTO,NUMBERS,AB,IL,ITEMP,ITEM,IT,TEMP,TEM,KET
COMMON NSUBST,EBUL,ETHERM,NSIDE,NBUL,NSAME,INTERST,INPAIRS,NFACE
COMMON ESIDE,NVAC,ECAL,OENERGY,NITEMP,DEPTH,PERDIST,IC,EPB
COMMON YENTRY,ZENTRY
EQUIVALENCE(LB,OCTAL)
DO 1320 I=1,3
1320 IB(I)=B(I,L)/A+0.5
ITEMP=IB(1)+IB(2)+IB(3)
IF(12*(ITEMP/2)-ITEMP) 1330,1325,1330
1325 IL=IB(3)*NPLANE+IB(2)*NLINE+IB(1)/2+1
RETURN
1330 NUMBERS(1)= IB(3) *NPLANE+ IB(2) *NLINE+(IB(1)+1)/2+1
NUMBERS(2)= IB(3) *NPLANE+ IB(2) *NLINE+(IB(1)-1)/2+1
NUMBERS(3)= IB(3) *NPLANE+(IB(2)+1)*NLINE+ IB(1) /2+1
NUMBERS(4)= IB(3) *NPLANE+(IB(2)-1)*NLINE+ IB(1) /2+1
NUMBERS(5)=(IB(3)+1)*NPLANE+ IB(2) *NLINE+ IB(1) /2+1
NUMBERS(6)=(IB(3)-1)*NPLANE+ IB(2) *NLINE+ IB(1) /2+1
TEMP=1.0E50
DO 1340 I=1,6
IT=NUMBERS(I)
AJP3(1340) SUB(MAXLAT)
AJP(1333) AJP2(1340)
1333 CALL INITIAL(IT)
TEM=C.0
DO 1335 ITEMP=1,3
FI(ITEMP)=XYZ(ITEMP)-B(ITEMP,L)
1335 TEM=TEM+FI(ITEMP)*FI(ITEMP)
IF(TEM-TEMP) 1337,1340,1340
1337 IL=IT
TEMP=TEM
1340 CONTINUE
END

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SUBROUTINE INITIAL(L)
DIMENSION AB(3),B(7,2370),FI(3),IB(3),LB(2370),XYZ(3),EMAX(30)
DIMENSION YENTRY(10),ZENTRY(10),OCTAL(2370),KET(26)
DIMENSION IHISTO(105),NUMBERS(50),MISTAKE(10)
DIMENSION NSIDE(6),ESIDE(6),NITEMP(10),IC(100),TSLI(30),NTSC(30)
COMMON IX,IY,IZ,FI,A,NLINE,NPLANE,LMAX,IB,LB,XYZ,MAXLAT,B,OCTAL
COMMON IHISTO,NUMBERS,AB,IL,ITEMP,ITEM,IT,TEMP,TEM,KET
COMMON NSUBST,EBUL,ETHERM,NSIDE,NBUL,NSAME,INTERST,INPAIRS,NFACE
COMMON ESIDE,NVAC,ECAL,OENERGY,NITEMP,DEPTH,PERCIST,IC,EPB
COMMON YENTRY,ZENTRY
EQUIVALENCE(LB,OCTAL)
IF(L-MAXLAT) 1003,1003,1023
1003 CONTINUE
IB(3)=(L-1)/NPLANE
STQ(ITEMP)
IB(2)=ITEMP/NLINE
STQ(ITEMP)
IB(1)=ITEMP*2
ITEMP=IB(2)+IB(3)
IF(2*(ITEMP/2)-ITEMP) 1005,1010,1010
1005 IB(1)=IB(1)+1
1010 DO 1015 I=1,3
FI(I)=IB(I)
1015 XYZ(I)=A*FI(I)
RETURN
1023 XYZ(1)=0.0
XYZ(2)=YENTRY(L-MAXLAT)
XYZ(3)=ZENTRY(L-MAXLAT)
END

```

BOX 14

```

SUBROUTINE ECCUNT(L)
DIMENSION AB(3),B(7,2370),FI(3),IB(3),LB(2370),XYZ(3),EMAX(30)
DIMENSION YENTRY(10),ZENTRY(10),OCTAL(2370),KET(26)
DIMENSION IHISTO(105),NUMBERS(50),MISTAKE(10)
DIMENSION NSIDE(6),ESIDE(6),NITEMP(10),IC(100),TSLI(30),NTSC(30)
COMMON IX,IY,IZ,FI,A,NLINE,NPLANE,LMAX,IB,LB,XYZ,MAXLAT,B,OCTAL
COMMON IHISTO,NUMBERS,AB,IL,ITEMP,ITEM,IT,TEMP,TEM,KET
COMMON NSUBST,EBUL,ETHERM,NSIDE,NBUL,NSAME,INTERST,INPAIRS,NFACE
COMMON ESIDE,NVAC,ECAL,OENERGY,NITEMP,DEPTH,PERDIST,IC,EPB
COMMON YENTRY,ZENTRY
EQUIVALENCE(LB,OCTAL)
TEMP=KET(25)
TEMP=B(7,L)-TEMP
ENI1(25) AJP2(25)
DO 20 I=1,24
TEMP=KET(I+1)
TEMP=TEMP-B(7,L)
AJP2(25)
20 CONTINUE
25 RAO1(IC+50)
END

```

BOX 15

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SUBRCUTINE DEPTH(L)
DIMENSION AB(3),B(7,2370),FI(3),IB(3),LB(2370),XYZ(3),EMAX(30)
DIMENSION YENTRY(10),ZENTRY(10),OCTAL(2370),KET(26)
DIMENSION IHISTO(105),NUMBERS(50),MISTAKE(10)
DIMENSION NSIDE(6),ESIDE(6),NITEMP(10),IC(100),TSLI(30),NTSC(30)
COMMON IX,IY,IZ,FI,A,NLINE,NPLANE,LMAX,IB,LB,XYZ,MAXLAT,B,OCTAL
COMMON IHISTO,NUMBERS,AB,IL,ITEMP,ITEM,IT,TEMP,TEM,KET
COMMON NSUBST,EBUL,ETHERM,NSIDE,NBUL,NSAME,INTERST,INPAIRS,NFACE
COMMON ESIDE,NVAC,ECAL,OENERGY,NITEMP,DEPTH,PERDIST,IC,EPB
COMMON YENTRY,ZENTRY
EQUIVALENCE(LB,OCTAL)
DEPTH=B(1,L)-XYZ(1)
I=1
1625 TEMP=I
      IF(TEMP-6.5)*A-DEPTH) 1630,1635,1635
1630 IF(I-29) 1631,1631,1635
1631 I=I+1
      GO TO 1625
1635 IC(I)=IC(I)+1
      PERDIST=SQRT((B(2,L)-XYZ(2))*2+(B(3,L)-XYZ(3))*2)
      I=1
1640 TEMP=I
      IF(4*PERDIST-TEMP*A) 1650,1645,1645
1645 I=I+1
      GO TO 1640
1650 IC(I+30)=IC(I+30)+1
      END

```

BOX 16

```

SUBRCUTINE HISTO(NGROUPS)
DIMENSION AB(3),B(7,2370),FI(3),IB(3),LB(2370),XYZ(3),EMAX(30)
DIMENSION YENTRY(10),ZENTRY(10),OCTAL(2370),KET(26)
DIMENSION IHISTO(105),NUMBERS(50),MISTAKE(10)
DIMENSION NSIDE(6),ESIDE(6),NITEMP(10),IC(100),TSLI(30),NTSC(30)
COMMON IX,IY,IZ,FI,A,NLINE,NPLANE,LMAX,IB,LB,XYZ,MAXLAT,B,OCTAL
COMMON IHISTO,NUMBERS,AB,IL,ITEMP,ITEM,IT,TEMP,TEM,KET
COMMON NSUBST,EBUL,ETHERM,NSIDE,NBUL,NSAME,INTERST,INPAIRS,NFACE
COMMON ESIDE,NVAC,ECAL,OENERGY,NITEMP,DEPTH,PERDIST,IC,EPB
COMMON YENTRY,ZENTRY
EQUIVALENCE(LB,OCTAL)
NTOTAL=0
NUMBIG=0
DO 1110 I=1,NGROUPS
NTOTAL=NTOTAL+NUMBERS(I)
IF(NUMBERS(I)-NUMBIG) 1110,1110,1108
1108 NUMBIG=NUMBERS(I)
1110 CONTINUE
PRINT 1109,NTOTAL
1109 FORMAT(/10X,17H100 PERCENT MEANSI5/)
TCTALN=NTOTAL
BIGNUM=NUMBIG
DO 1113 J=1,NGROUPS
FNUMBER=NUMBERS(J)
NUMBER=100.0*FNUMBER/BIGNUM+0.5
TEMP=100.0*FNUMBER/TCTALN
DO 1111 I=5,104
1111 IHISTO(I)=3H1H
      ITEM=NUMBER+4
DO 1112 I=5,ITEMP
1112 IHISTO(I)=3H1HX
      IT=J+IL
1113 PRINT IHISTO,IT,TEMP
      END
END

```

```

PROGRAM RON
DIMENSION AB(3),B(3,2370),NT(2000),P(3),X(3,2000),S(3)
DIMENSION IB(3),FI(3),XYZ(3),NUMBERS(6),YENTRY(10),ZENTRY(10)
+SLJ1(L+1) SLJ(4)
IT=-1
WRITE TAPE 6,IT,IT,IT,IT
4 REWIND 6
PRINT 3
3 FORMAT(1H1)
PRINT 1
1 FORMAT(///// )
DO 5 I=1,6
READ INPUT TAPE 2,2
2 FORMAT(80H
1
5 PRINT 2
PRINT 1
SLJ2(7)
READ TAPE 6,IX,IY,IZ,AB,MAXLAT,A,SPHI,FMASS,ETHRESH,THERMAL,MNP
READ TAPE 6,((B(I,J) I=1,3) J=1,MAXLAT),NLINE,NPLANE
PRINT 1098,IX,AB(1),IY,AB(2),IZ,AB(3),MAXLAT,A,SPHI,FMASS,ETHRESH,
1THERMAL
1098 FORMAT(29H THE LATTICE DIMENSIONS ARE -5X,11HX-DIRECTIONI6, 6H
1 X A =F11.7,10H ANGSTROMS/34X, 11HY-DIRECTIONI6,6H X A =F11.7, 1CH
2 ANGSTROMS/34X, 11HZ-DIRECTIONI6,6H X A =F11.7,10H ANGSTRCMS// 21H
3 THE LATTICE CONTANIS15,6H ATOMS//33H THE LATTICE SPACING CONSTANT
4 A =F10.7,10H ANGSTROMS/27H THE SPHERE CF INFLUENCE ISF16.7, 10H
5 ANGSTROMS/ 19H THE ATOMIC MASS ISF24.7,4H AMU//
6 4CH THRESHOLD ENERGY FOR VACANCY PRODUCTIONF10.3,4H EV./
7 25H THERMAL THRESHOLD ENERGYF25.3,4H EV.)
PRINT 1
LMAX=MAXLAT+MNP
7 READ INPUT TAPE 2,8,T
8 FORMAT(20X,F10.6)
DX=T*A
RA=1.0/A
ENI6(18)
10 READ TAPE 6,IT,P
LDA(IT) AJP3(30) LIU5(IT) SIL5(IN) LIL4(IT) SIL4(IL)
DO 15 I=1,3
T=ABSF(P(I)-B(I,IL))
FSB(DX) AJP2(20)
15 CONTINUE
SLJ(10)
20 DO 25 I=1,3
B(I,IL)=P(I)
25 X(I,N)=P(I)
LDA(IT) STA6(NT) +ISK6(3000) SLJ(10) ENI6(3001)
30 INI6(-1) SIL6(ITEMP) ENI2(08)
DO 45 L=1,LMAX
ENI5(08) SIL4(IL) ENA(-1) STA(NO)
DO 45 K=1,ITEMP
LDA3(NT) STA(IU) LIL1(IU) SIL1(II) LDA(II) SUB(IL)
AJP1(45) LIU1(IU) SIL1(IN) LDA(NO) AJP3(32) +ISK5(4) SLJ(42)
PRINT 41
41 FORMAT(/)
LDA(NO) AJP2(42)
32 PRINT 35,IL
35 FCRMAT(//1X ,20HORBIT OF ATOM NUMBERIS//
110H NUMBER OF9X,15HACTUAL POSITION16X,9HNUMBER OF7X,19HNORMALIZED
3POSITION/10H TIME STEP6X,1HX9X,1HY9X,1HZ13X,9HTIME STEP6X,1HXSX,
41HY9X,1HZ/)
INI2( 6)
NO=1
42 DO 40 I=1,3
40 S(I)=RA*X(I,K)
PRINT 43,IN,(X(I,K) I=1,3),IN,(S(I) I=1,3)
43 FORMAT(17,F13.4,2F10.4,116,F13.4,2F10.4,19)
45 CONTINUE
LDA(IT) AJP3(50) ENI6(18) SLJ(10)
50 CONTINUE
END
END

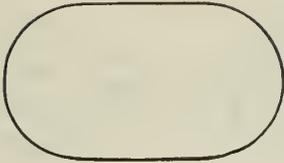
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APPENDIX IV
PROGRAM FLOW CHARTS

SYMBOLS USED IN THIS APPENDIX



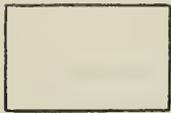
START of a program, subroutine, box, or page



Read in or write out



Decision or branch



General other computer operation



Position designation

[IJK • LMN]

Logical product of IJK and LMN

(A)

Contents of the "A register"

(Q)

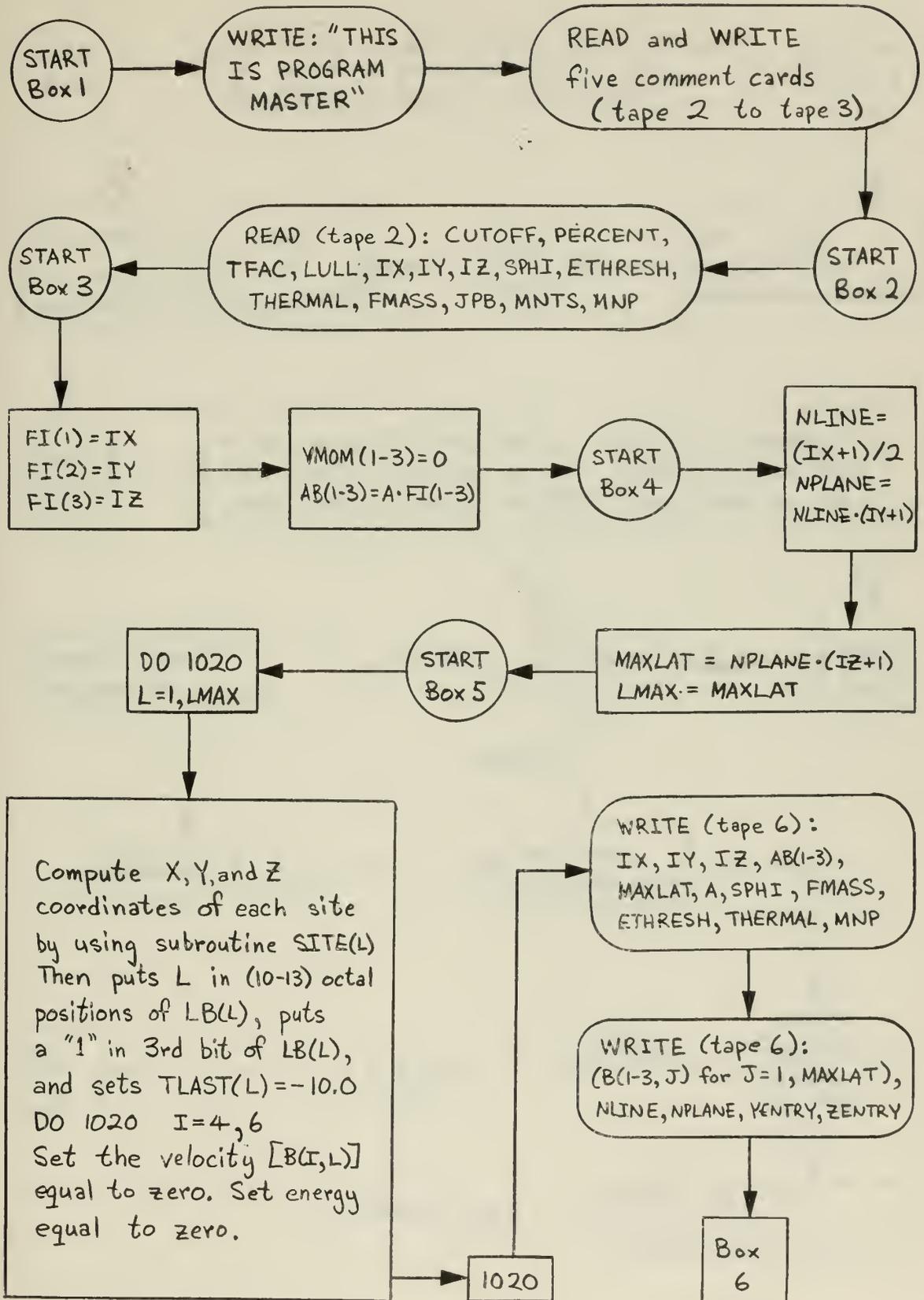
Contents of the "Q register"

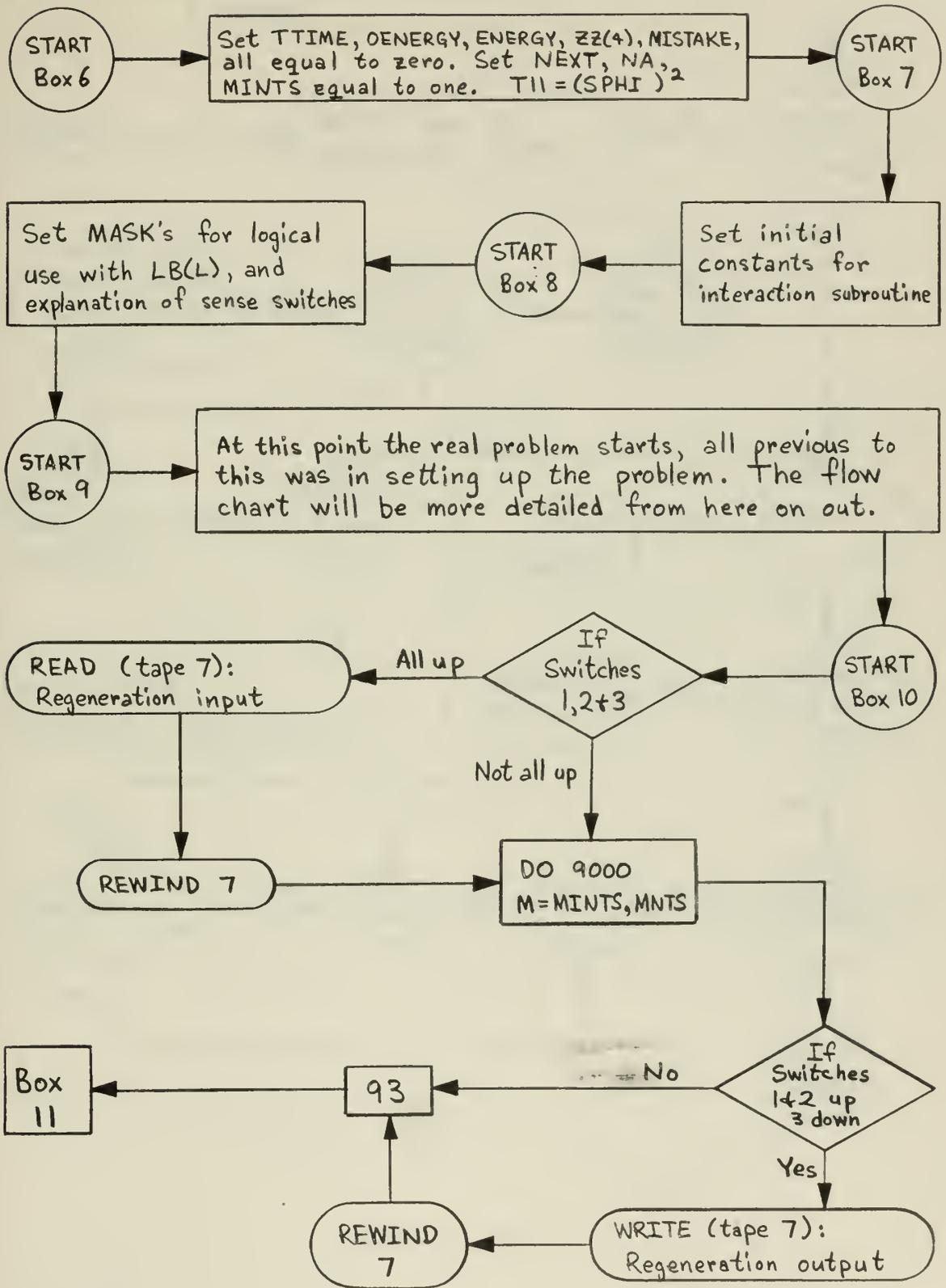
732

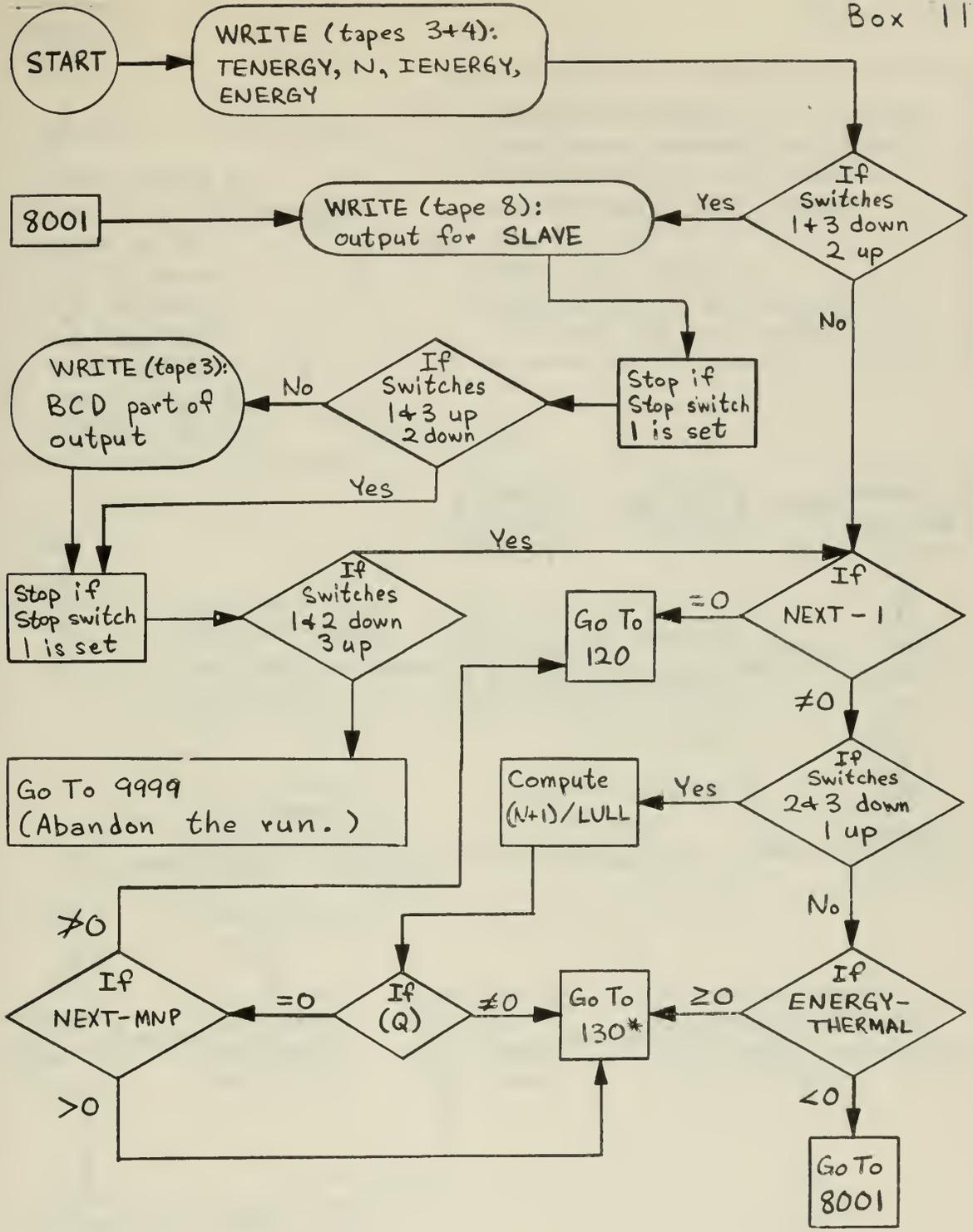
Statement number 732

PROGRAM MASTER

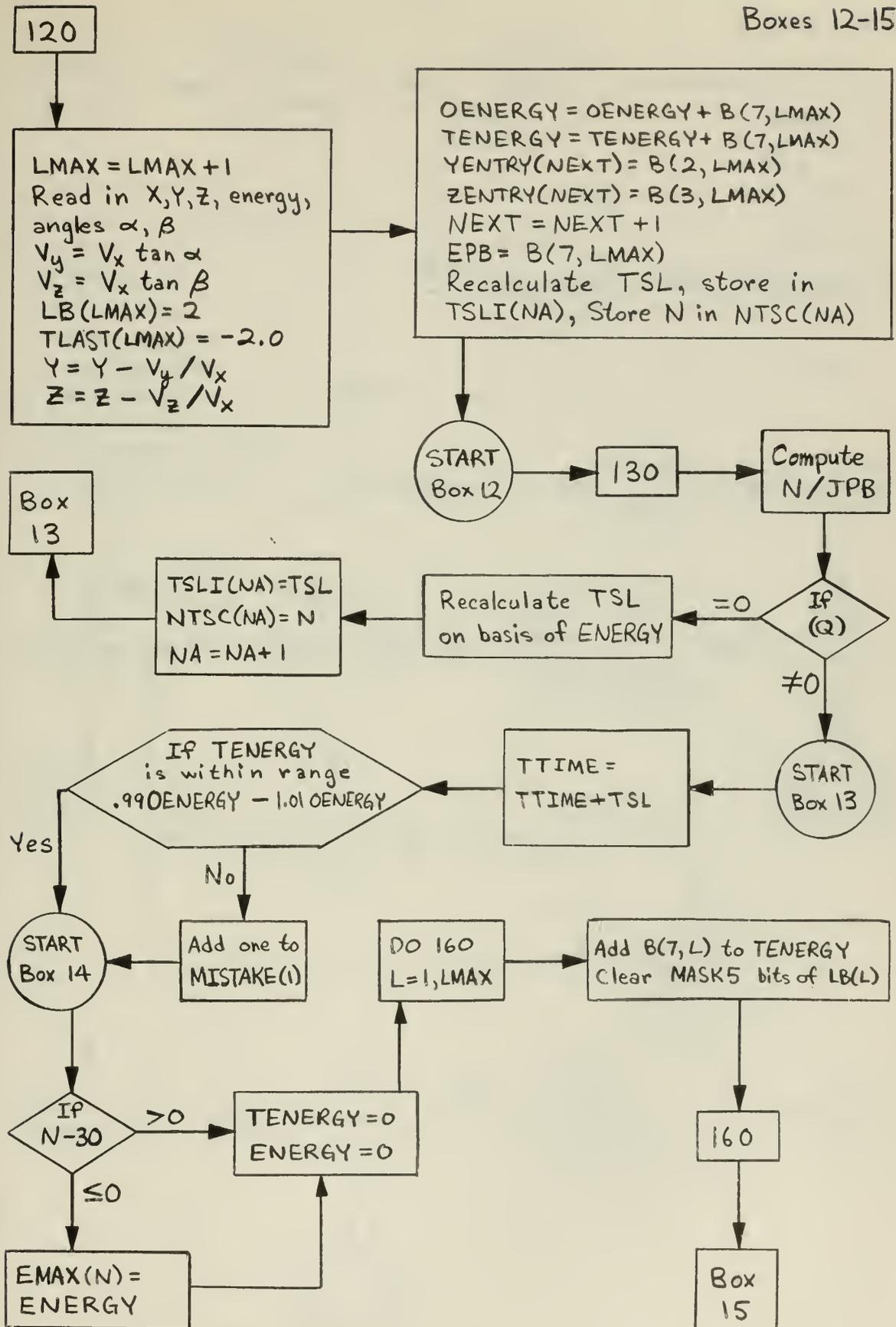
Boxes 1-5

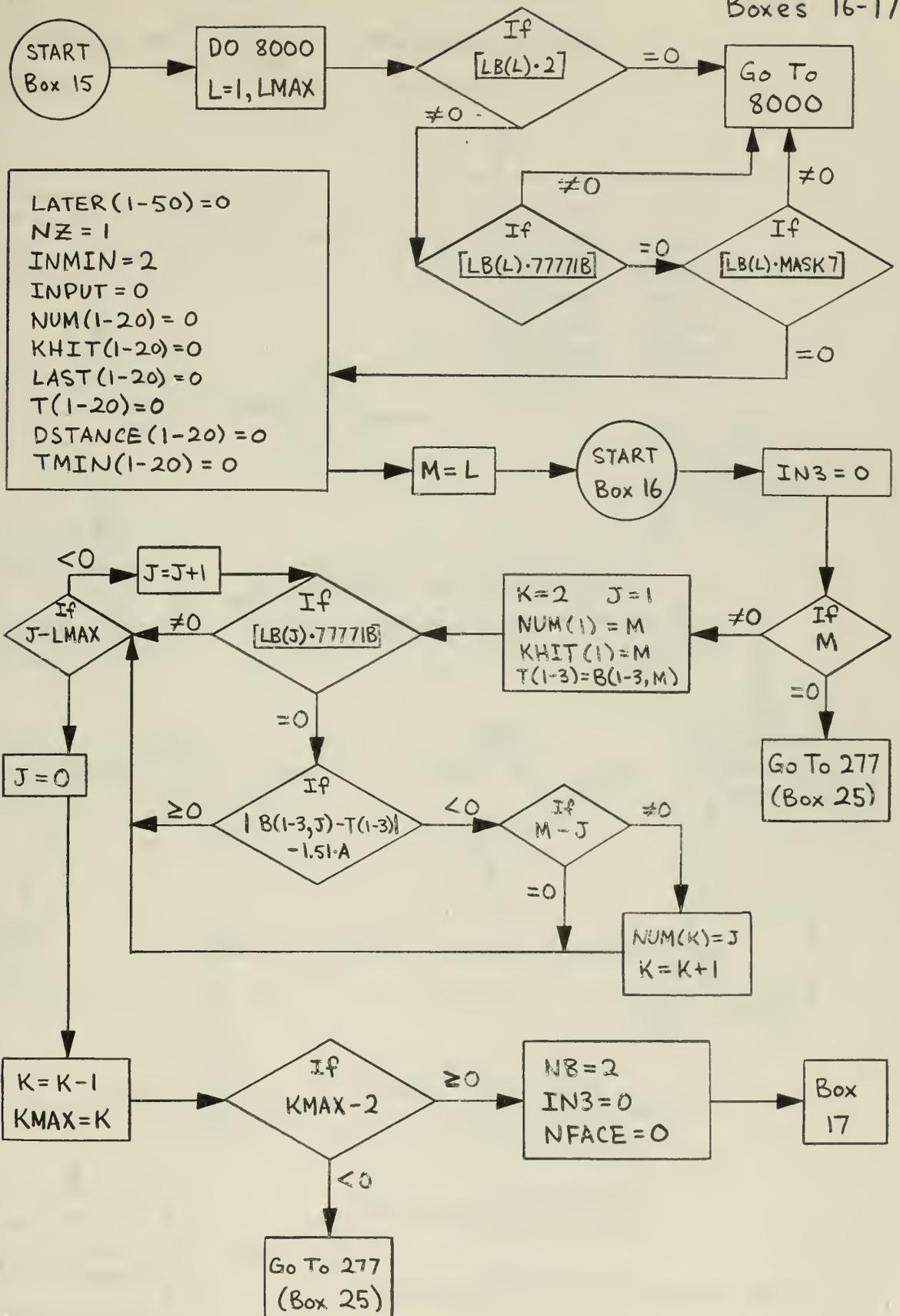


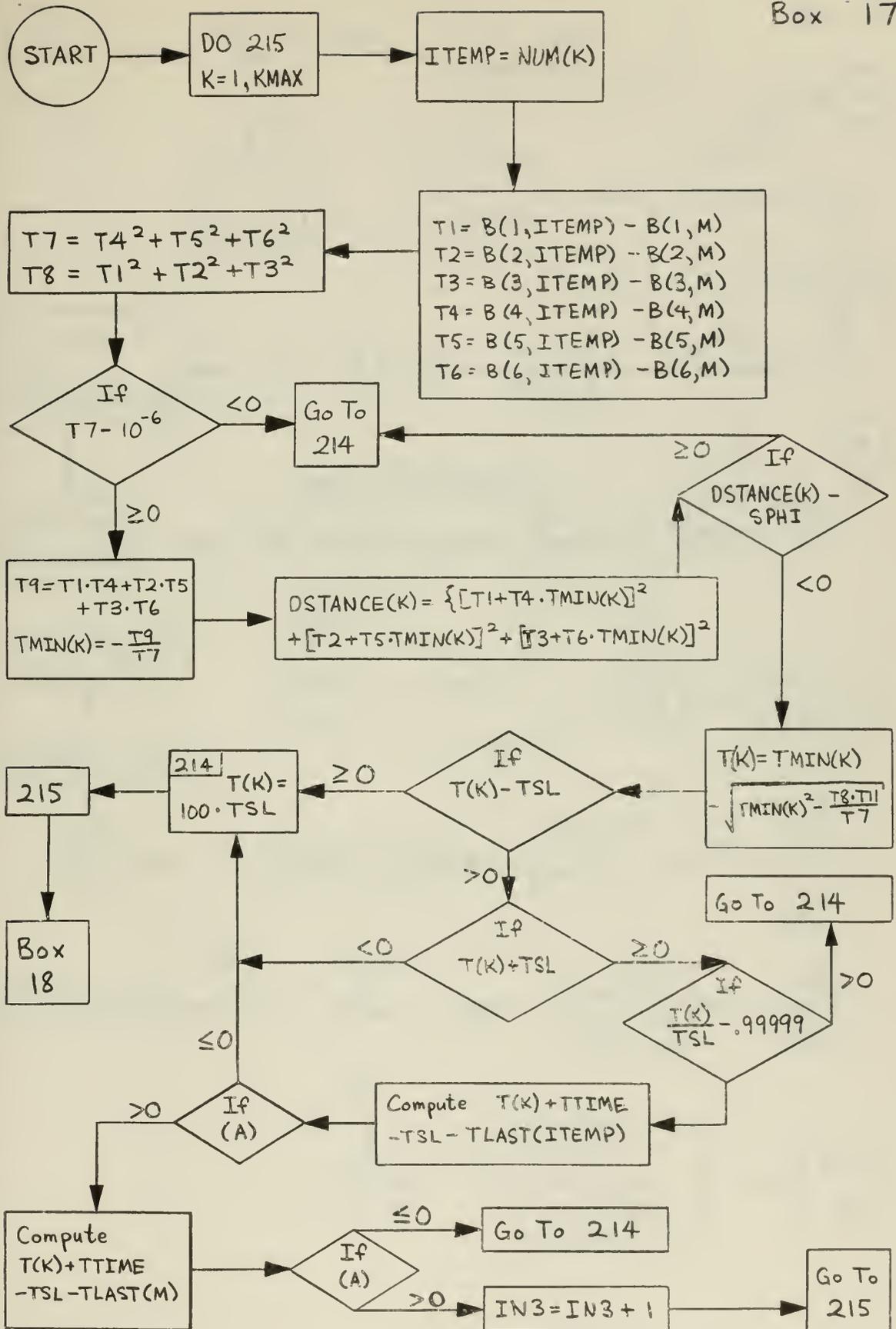


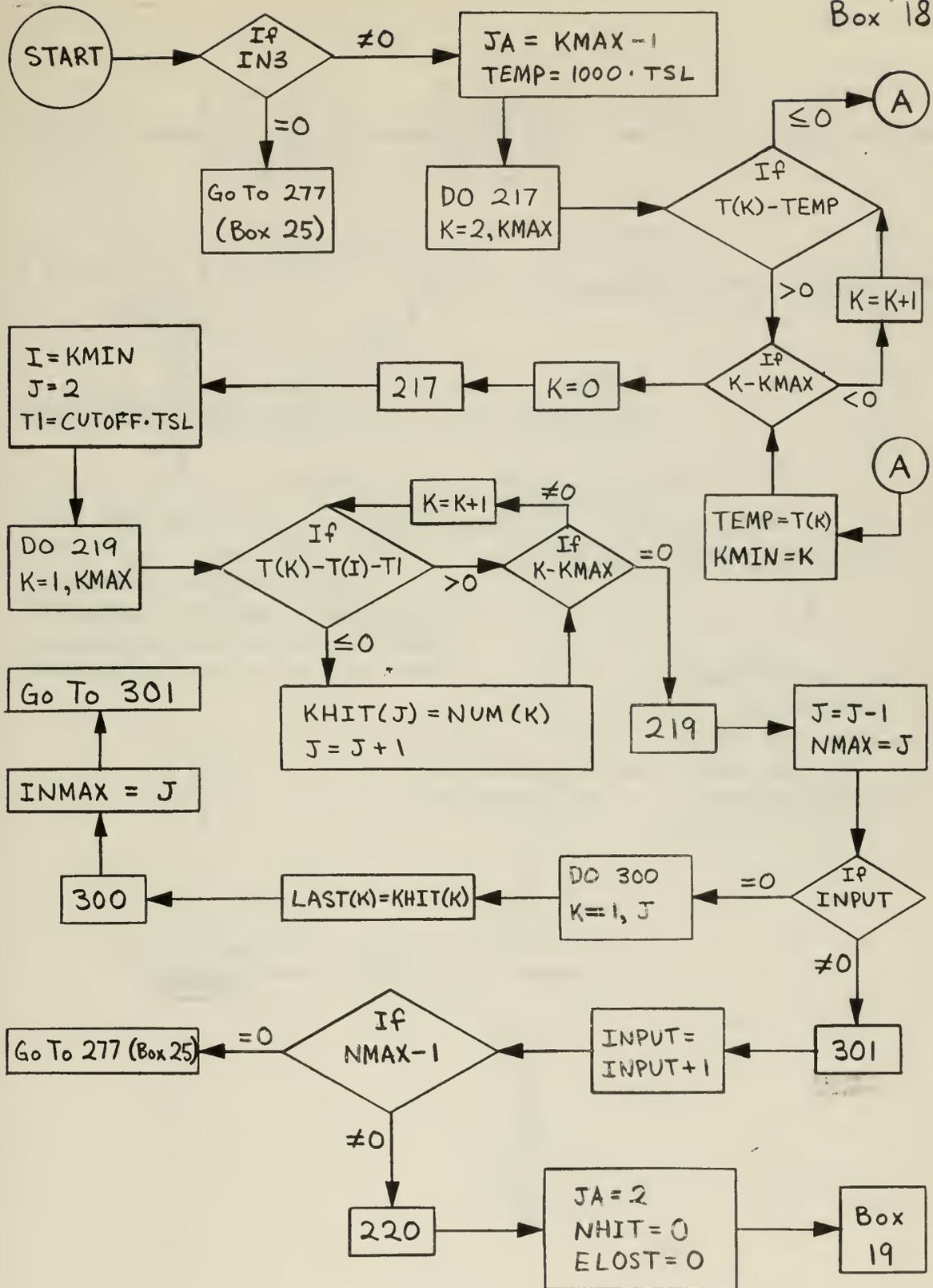


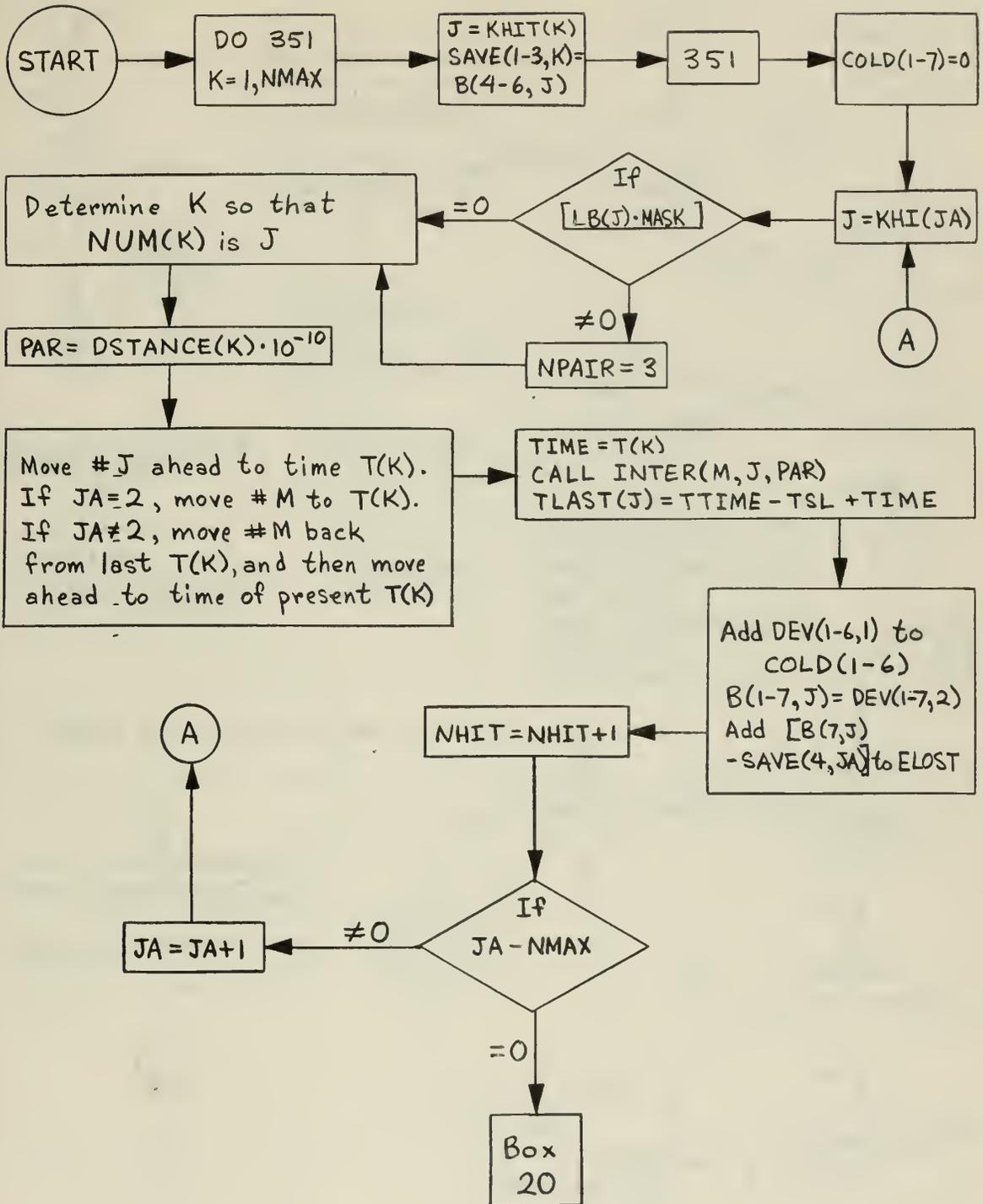
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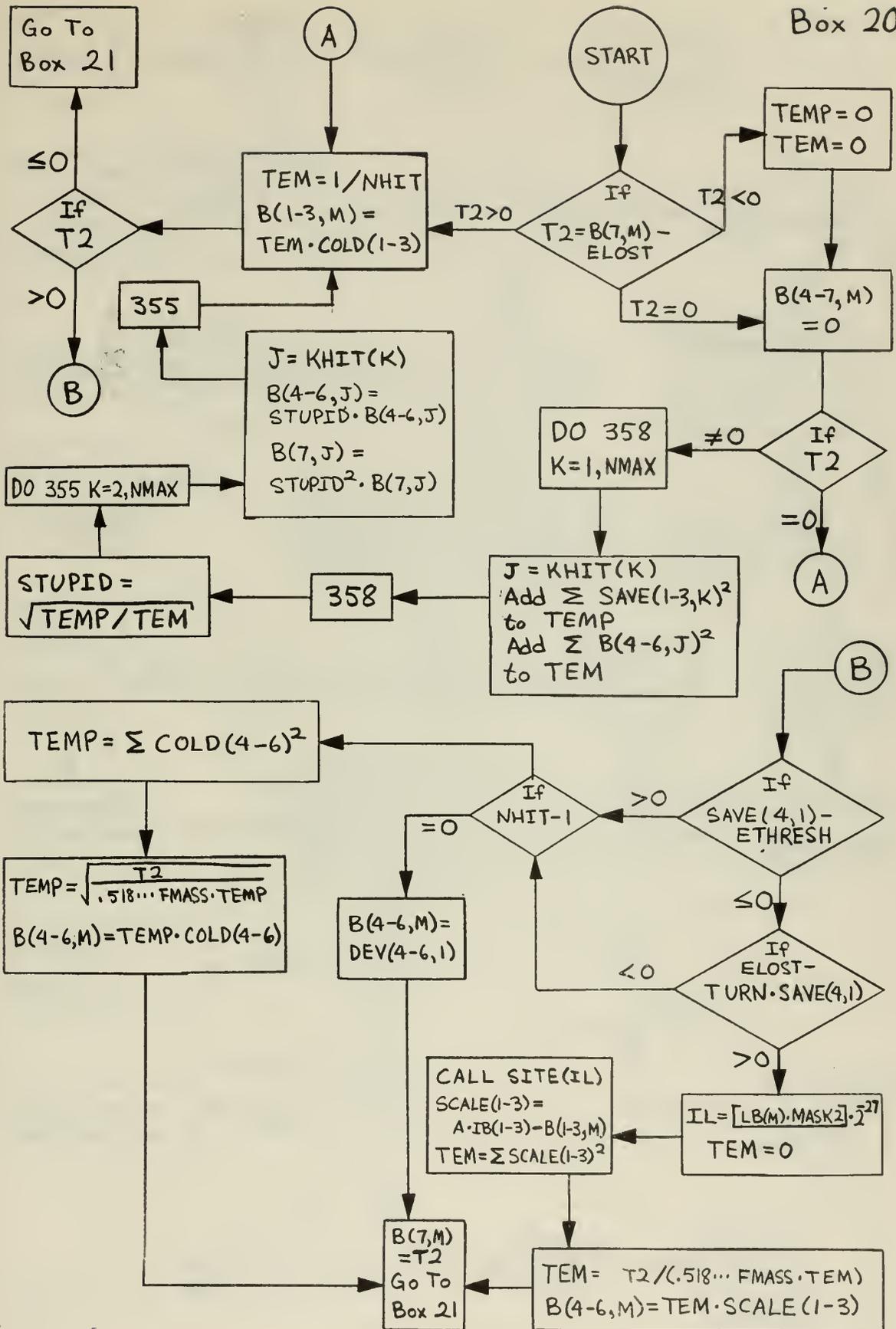


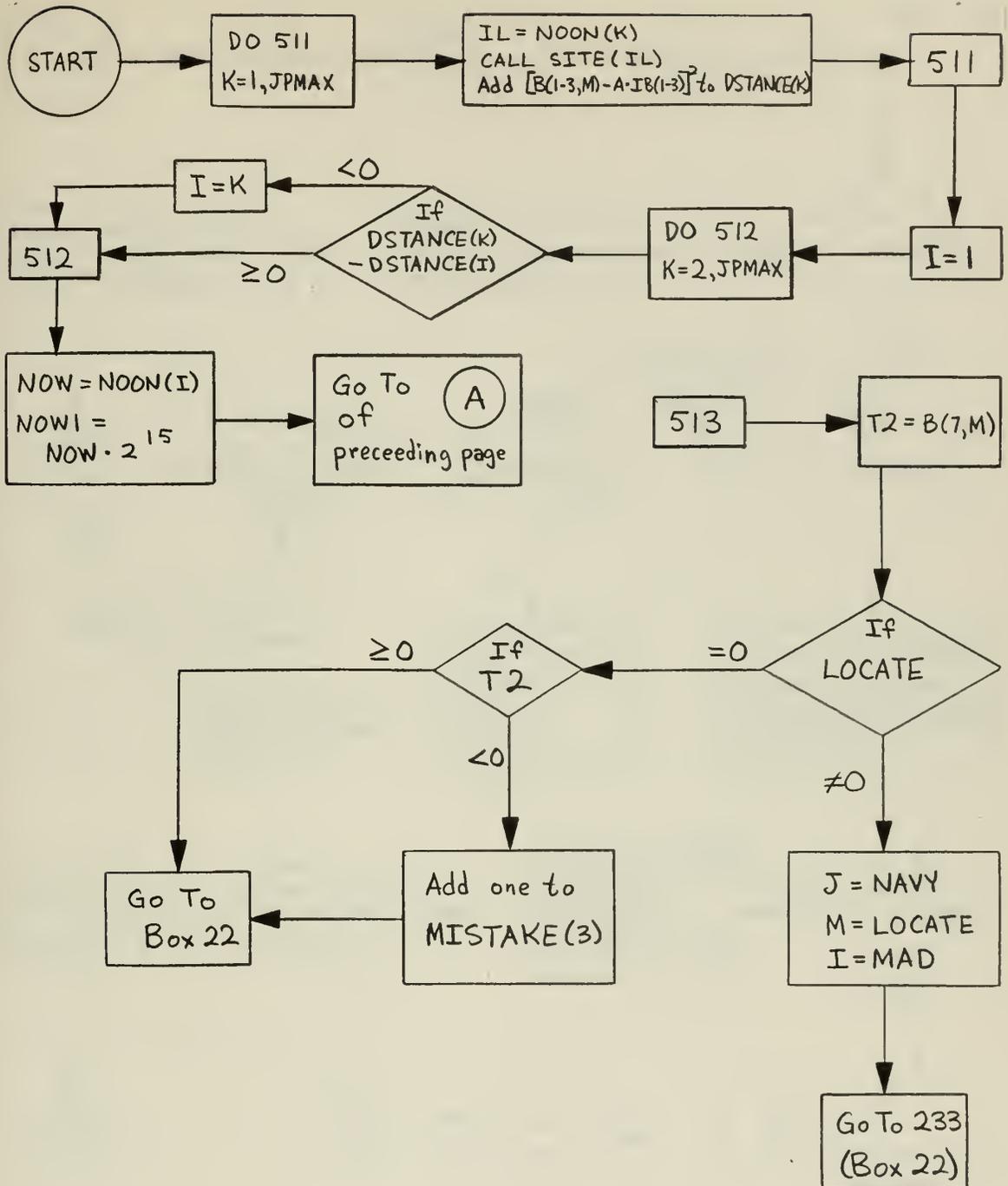


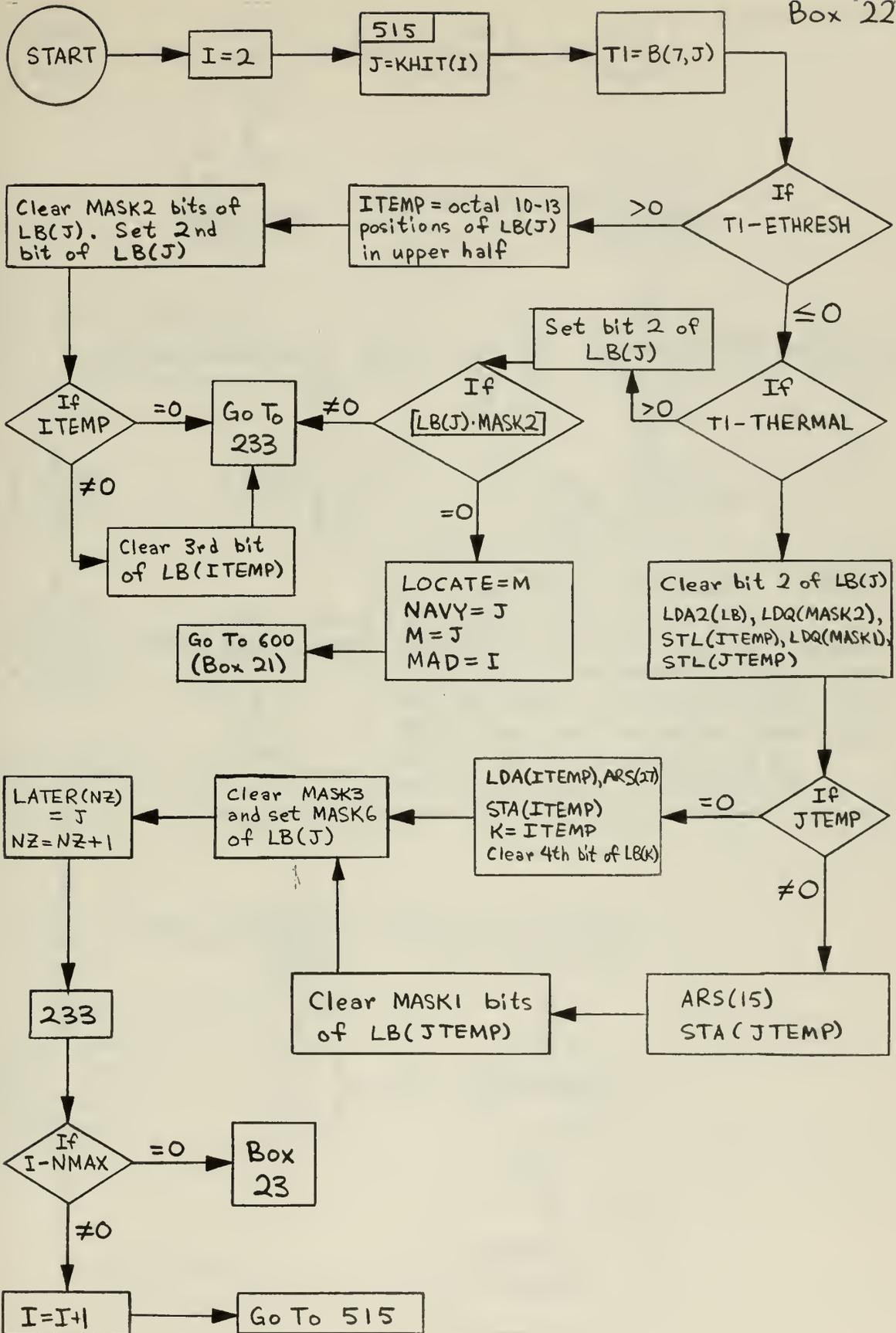


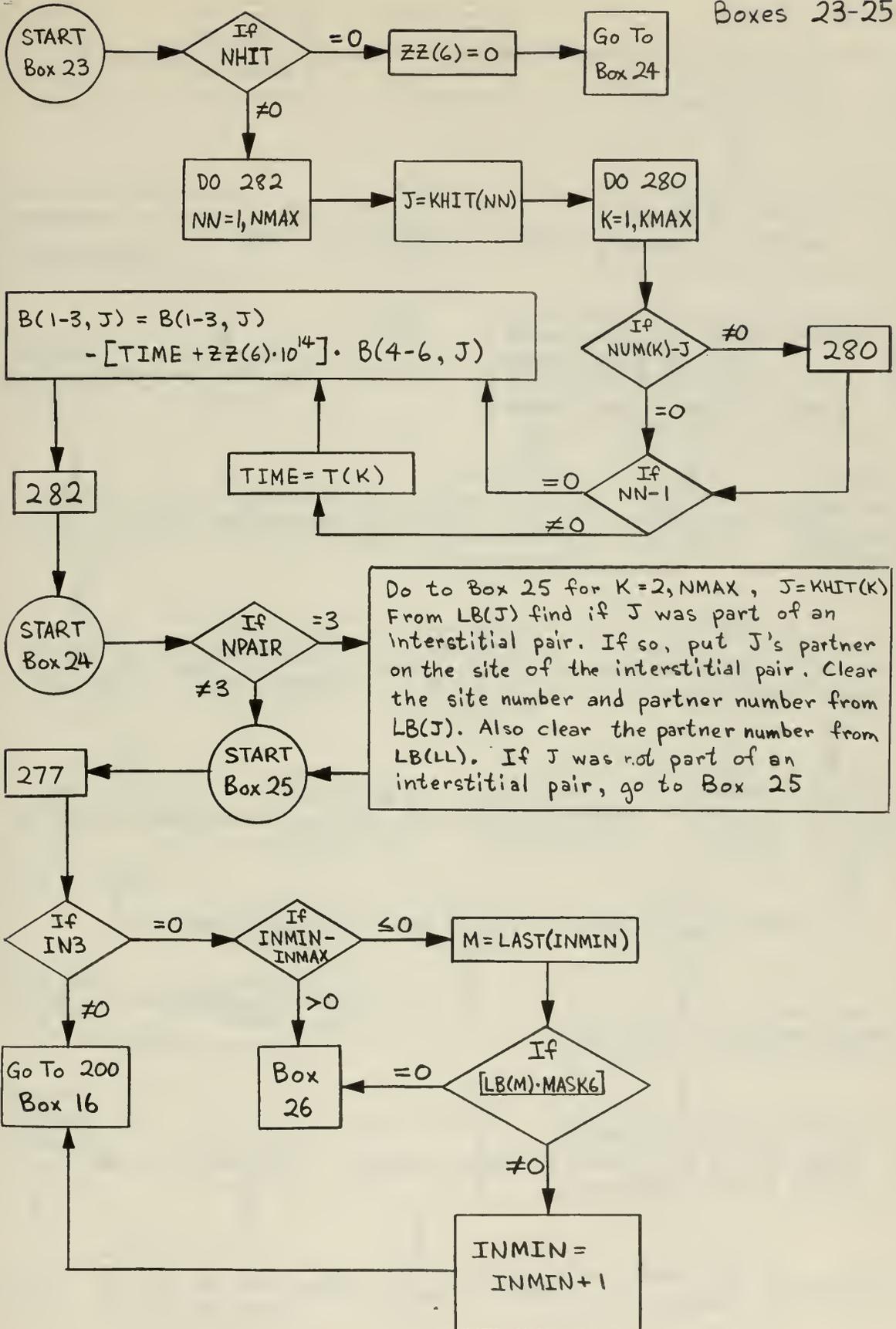


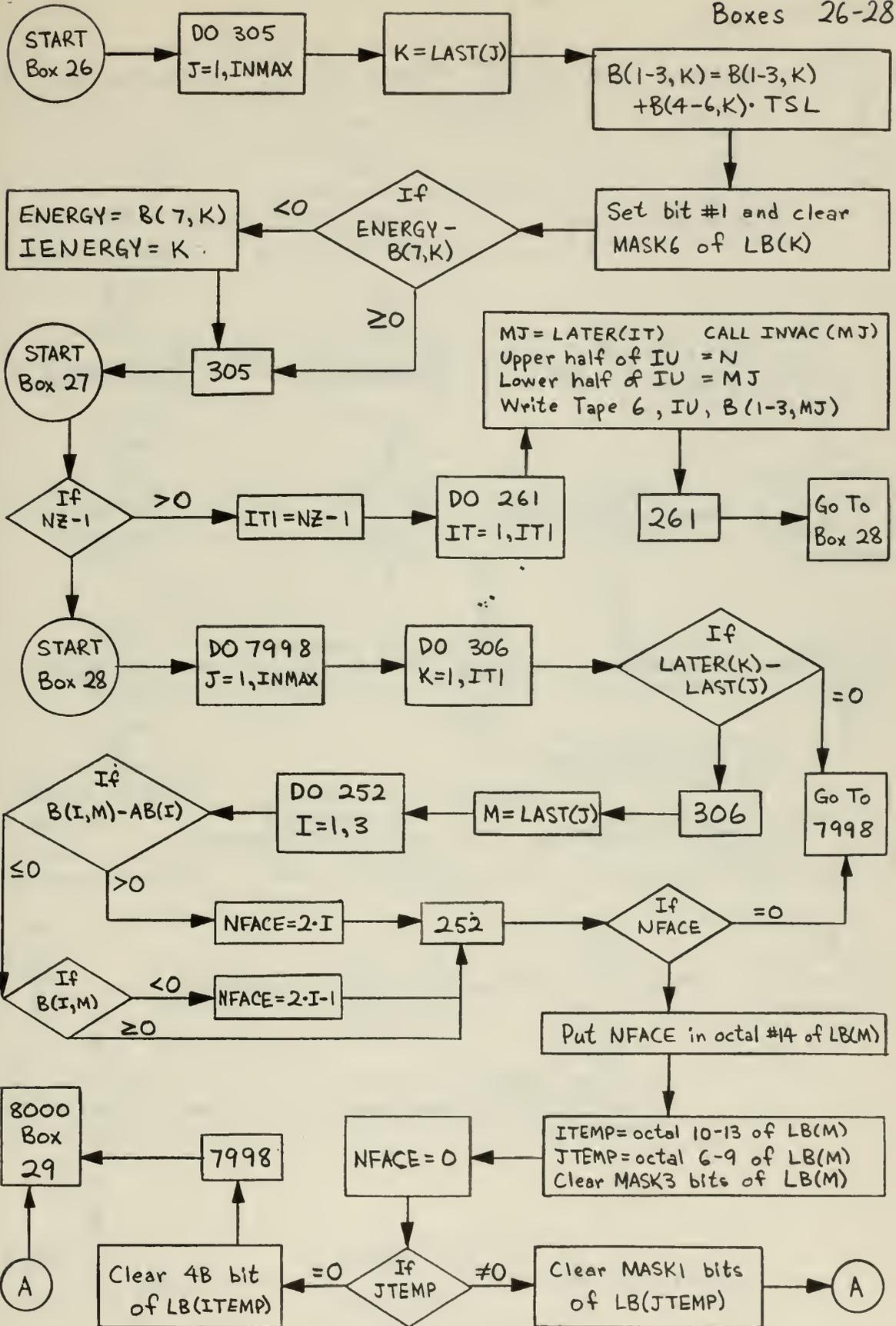


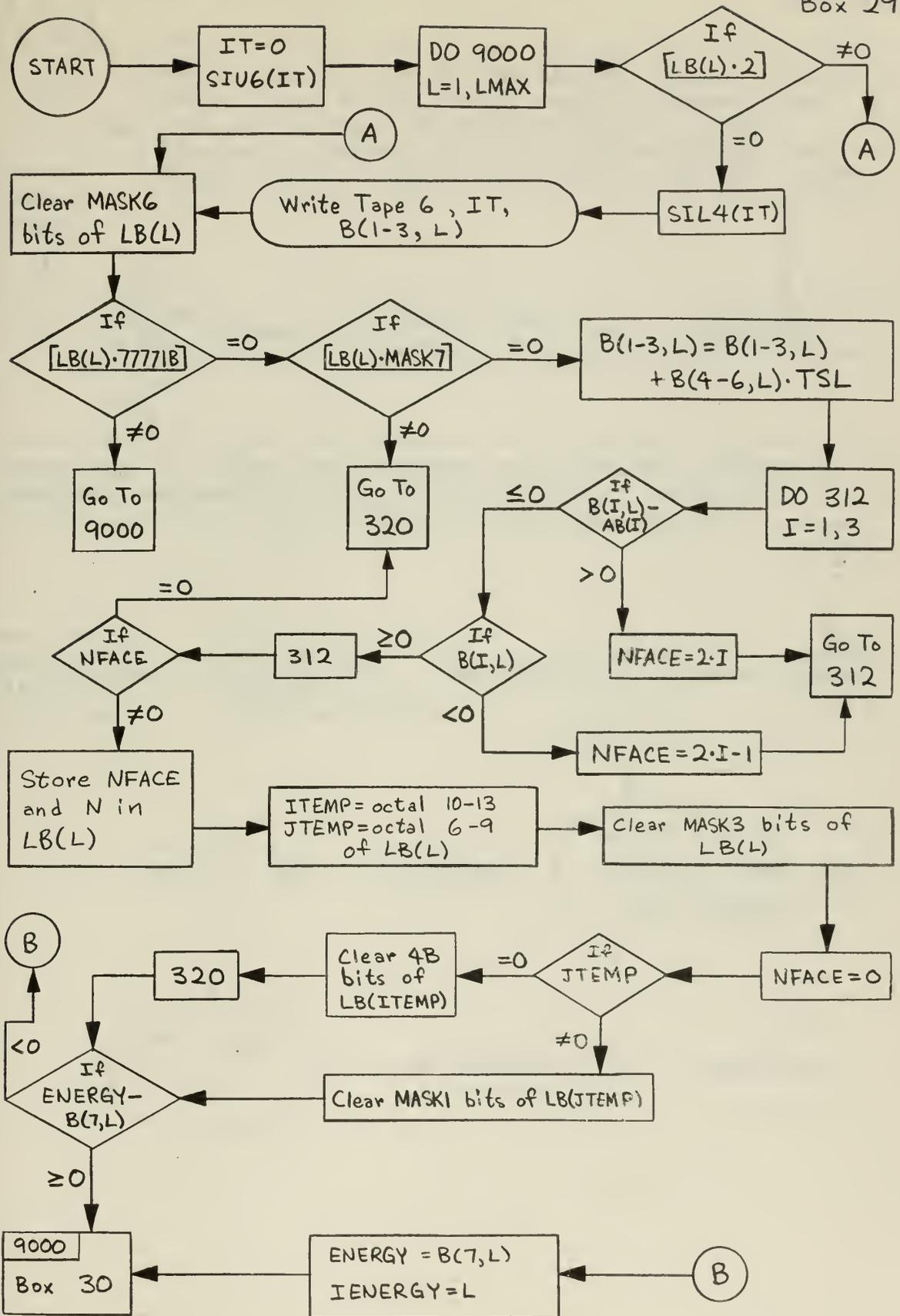


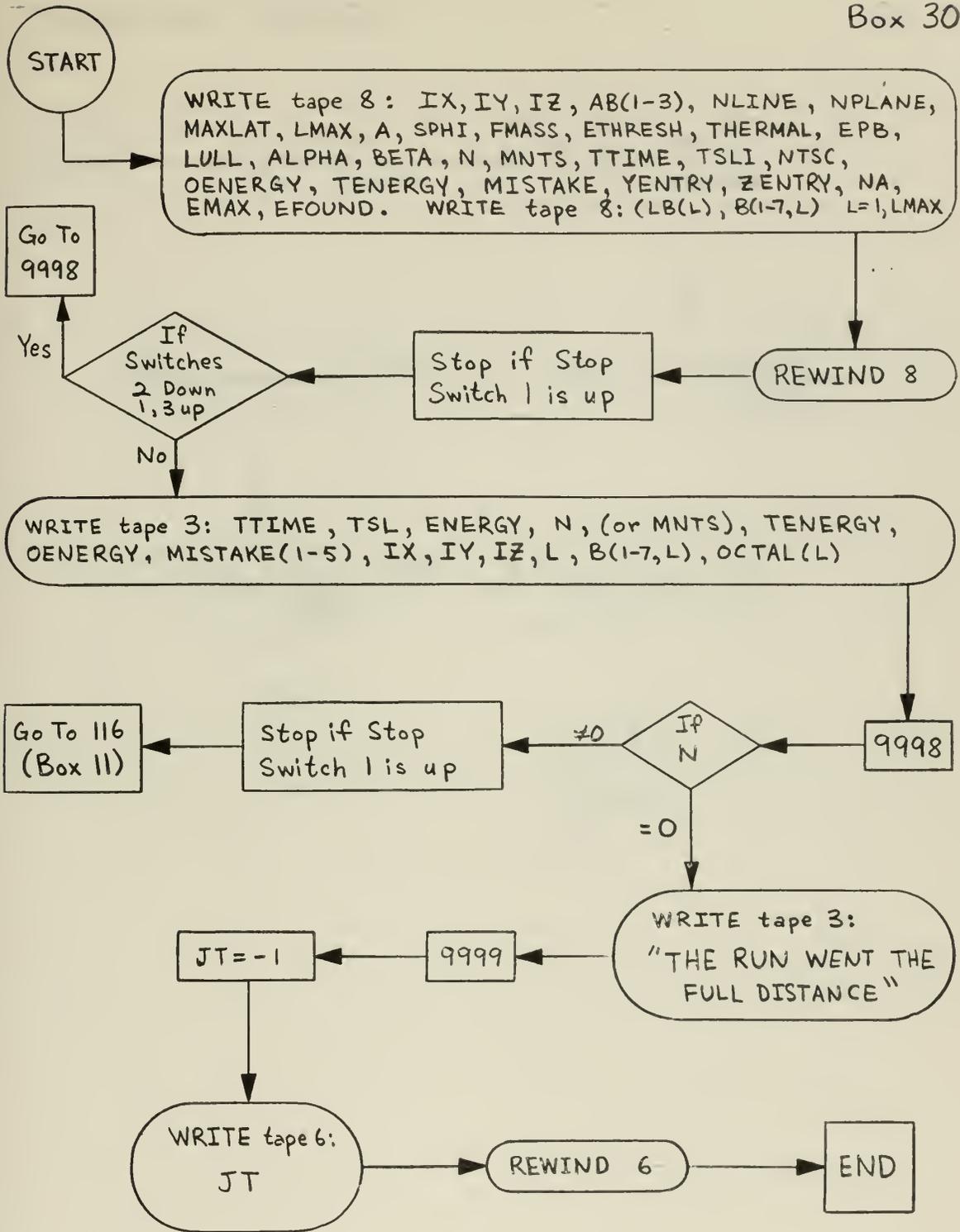


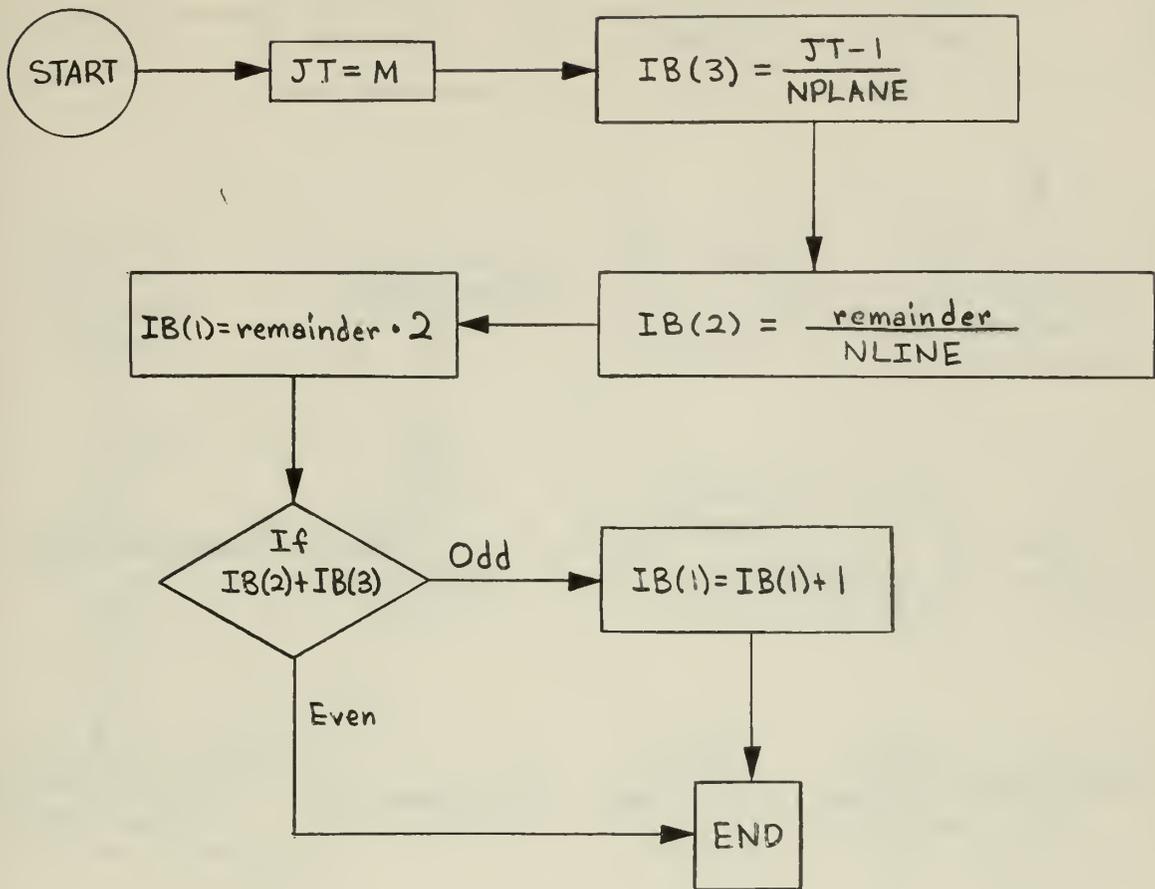


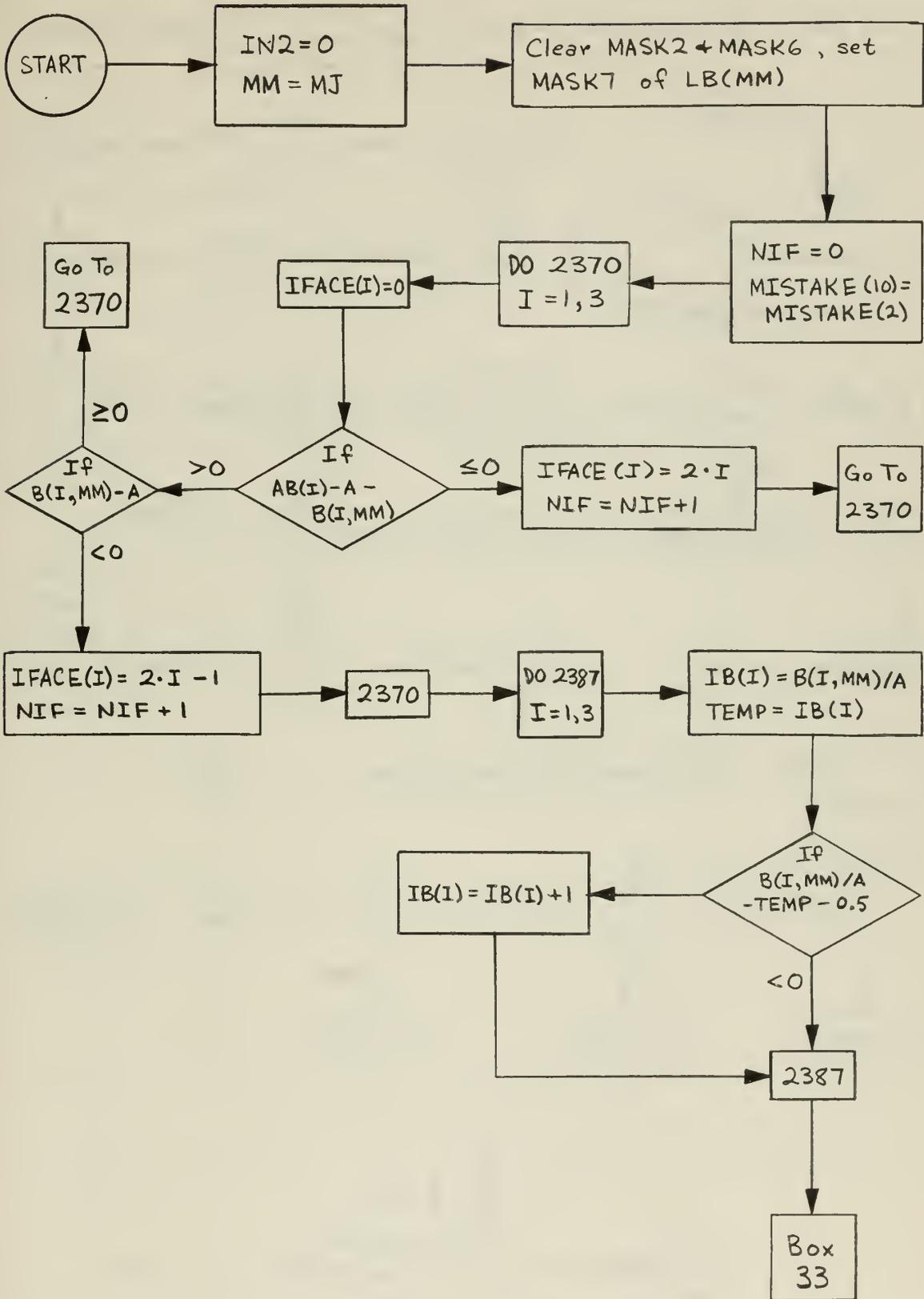


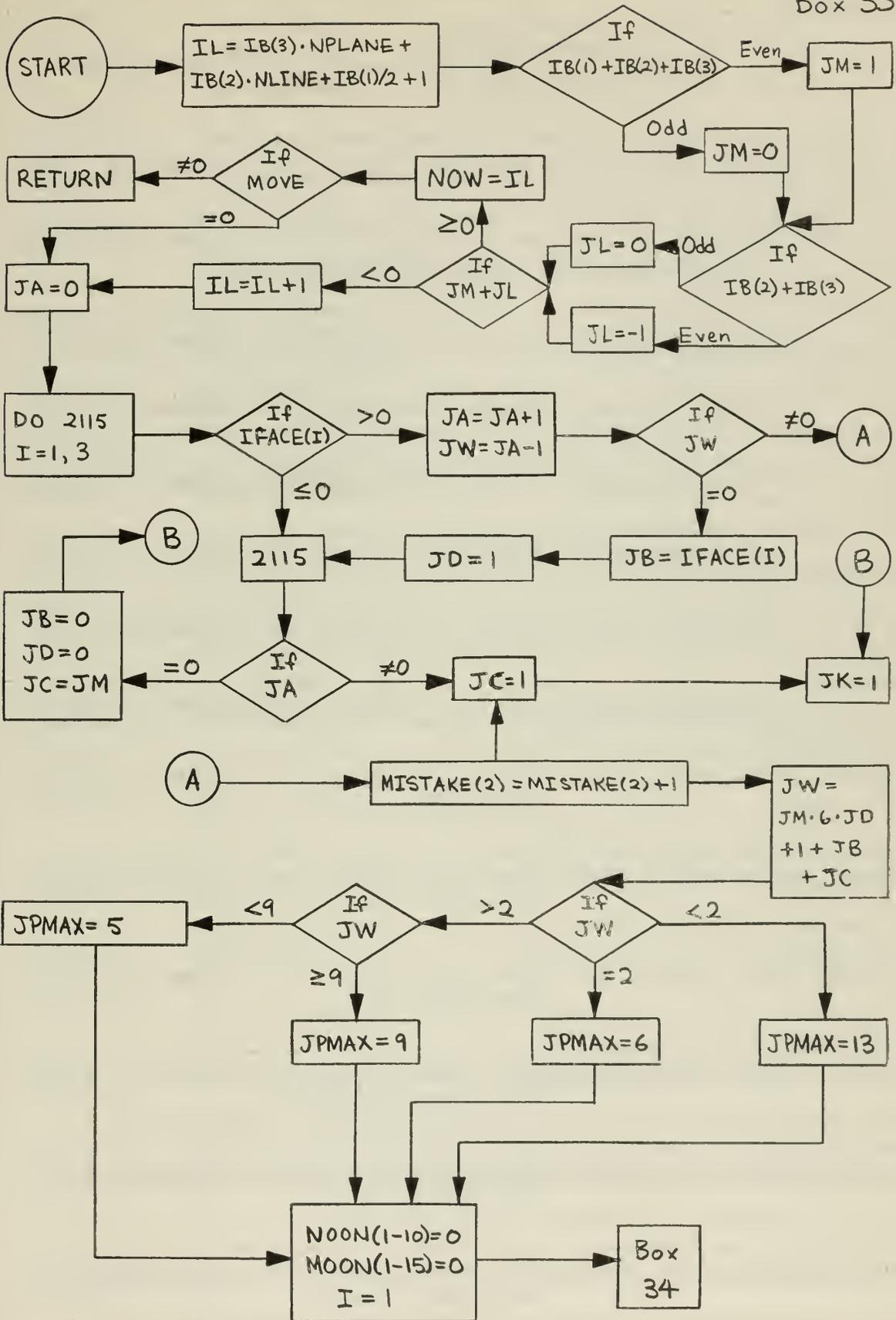


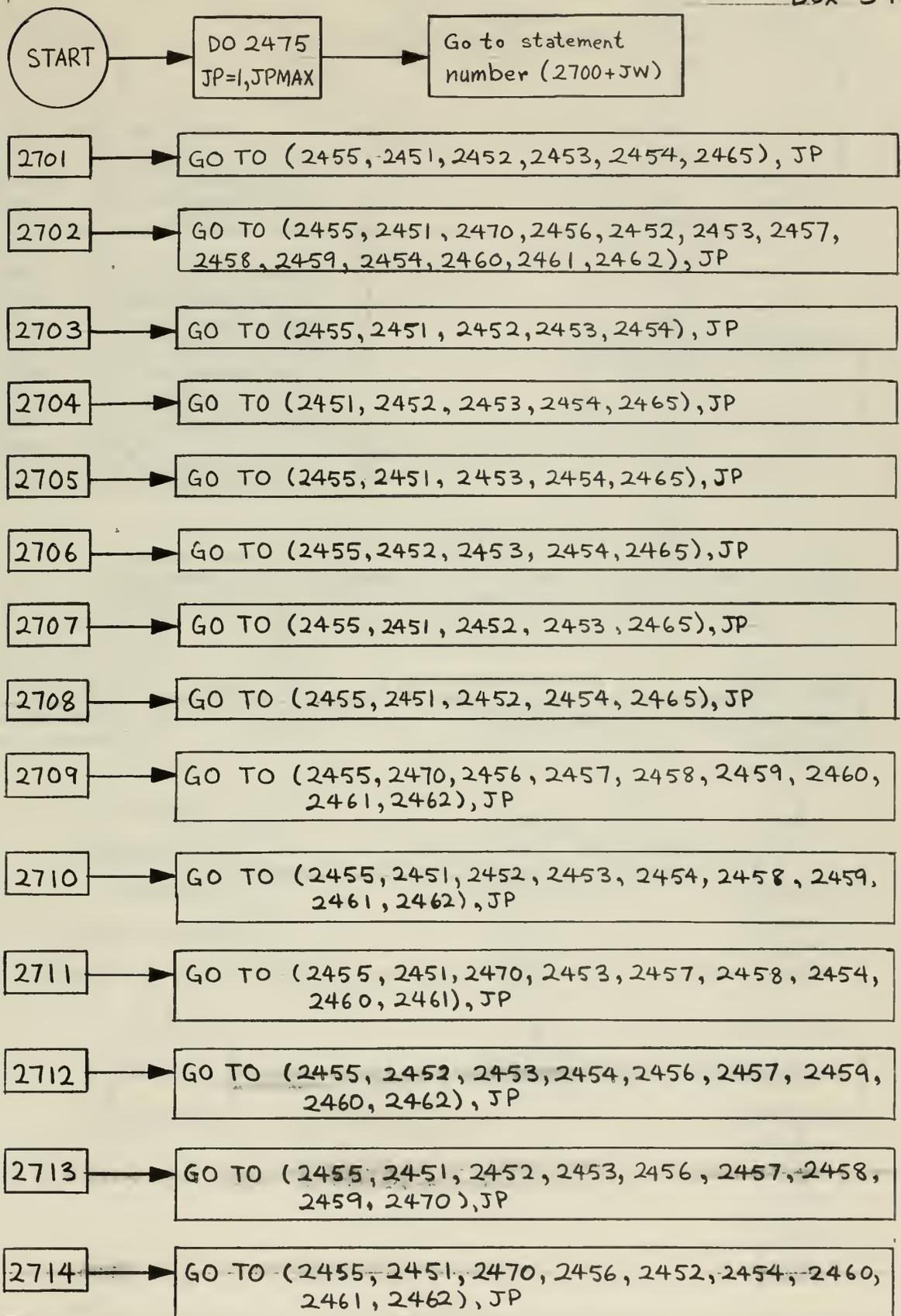


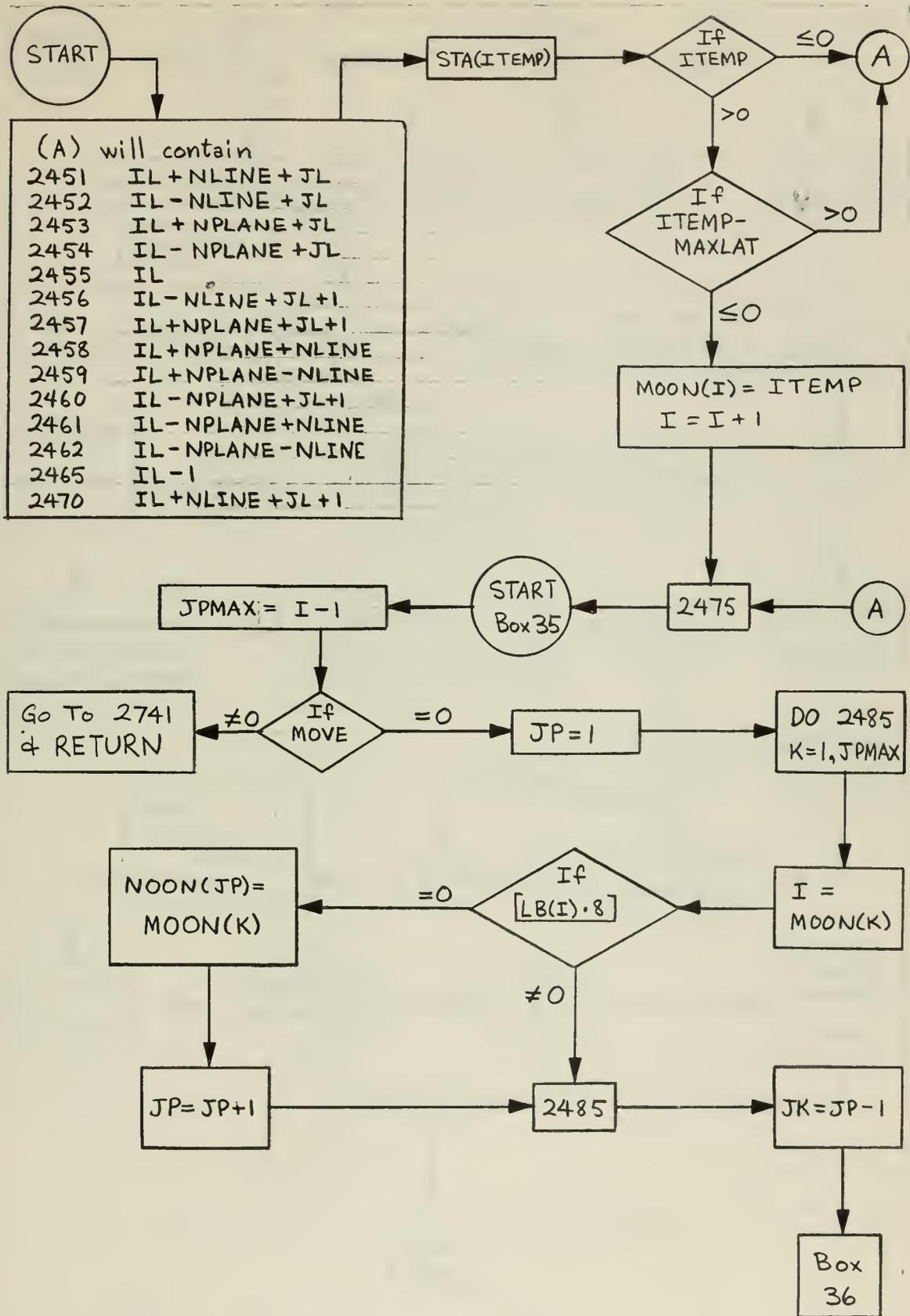


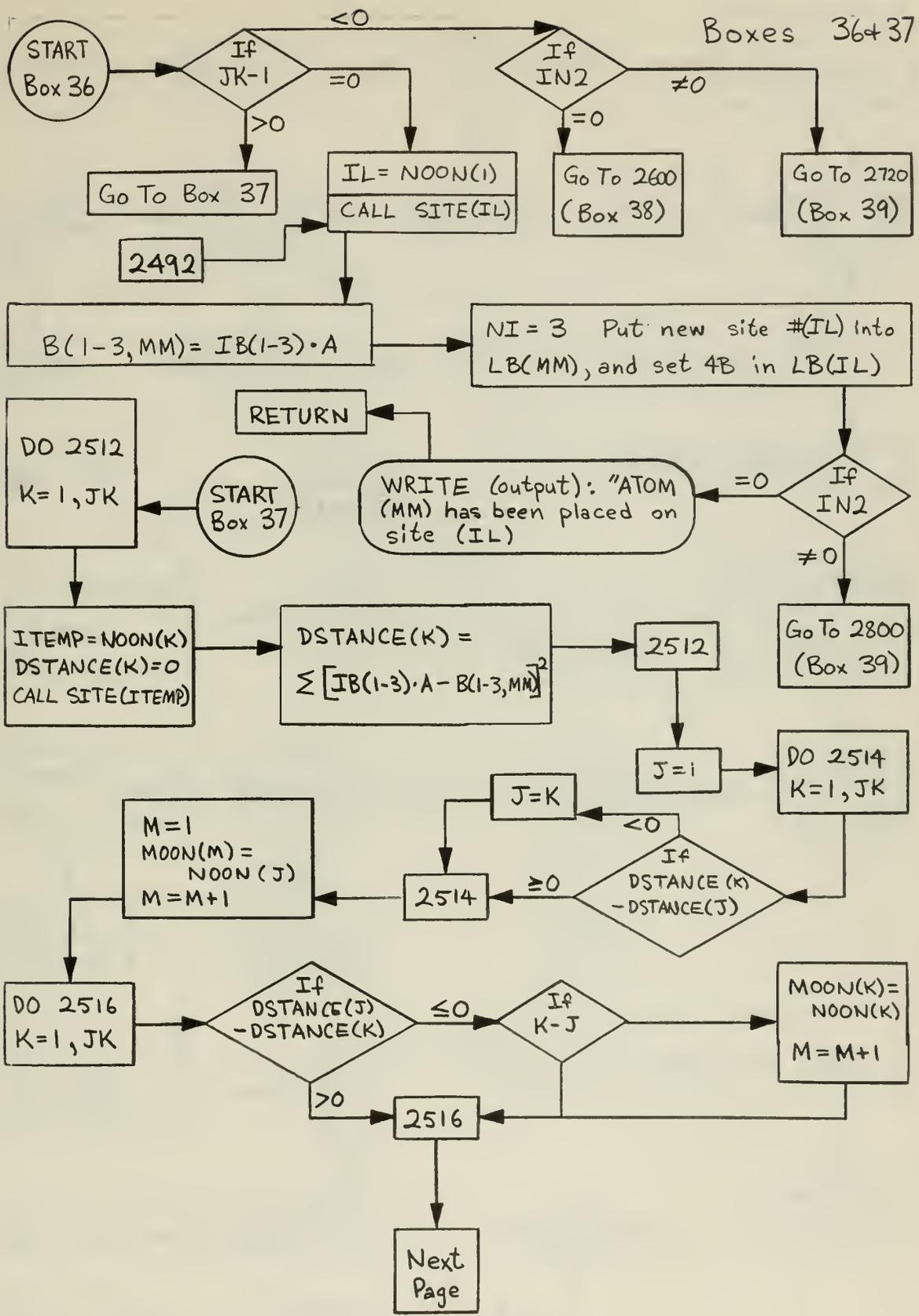


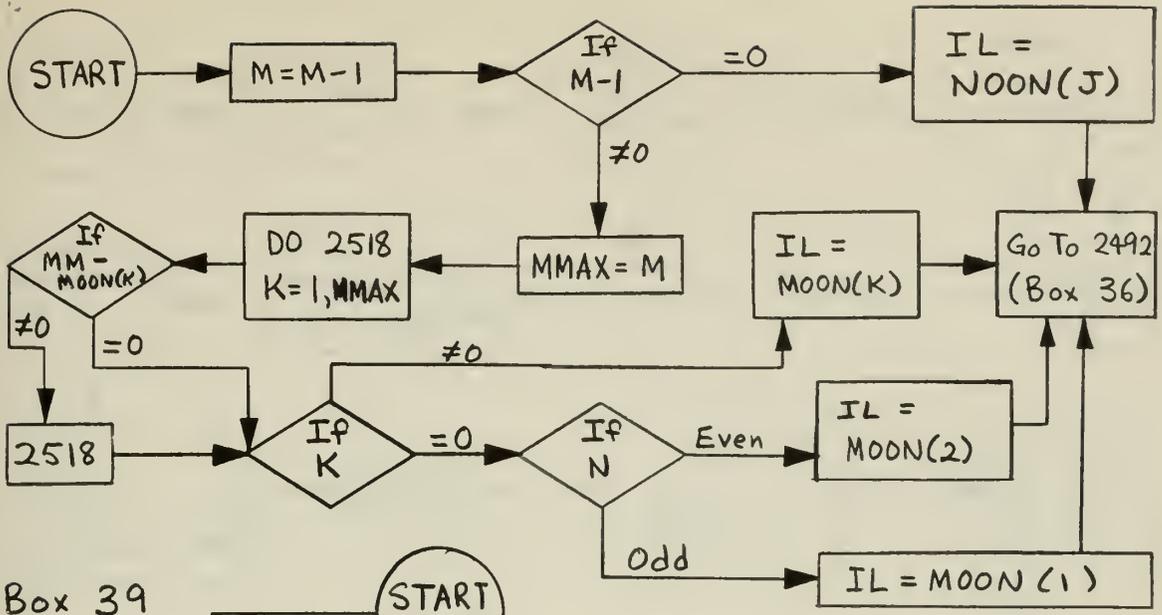




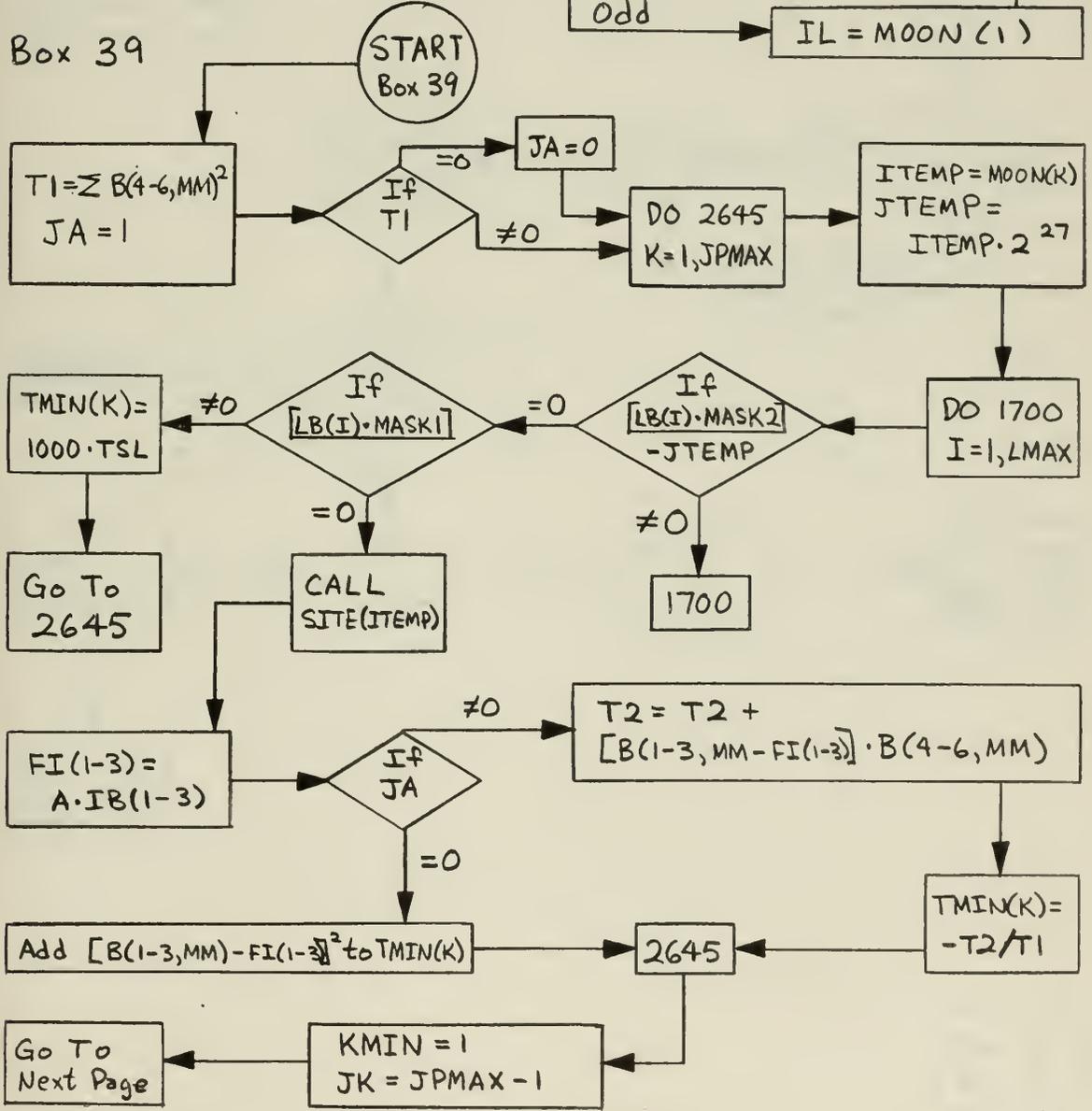


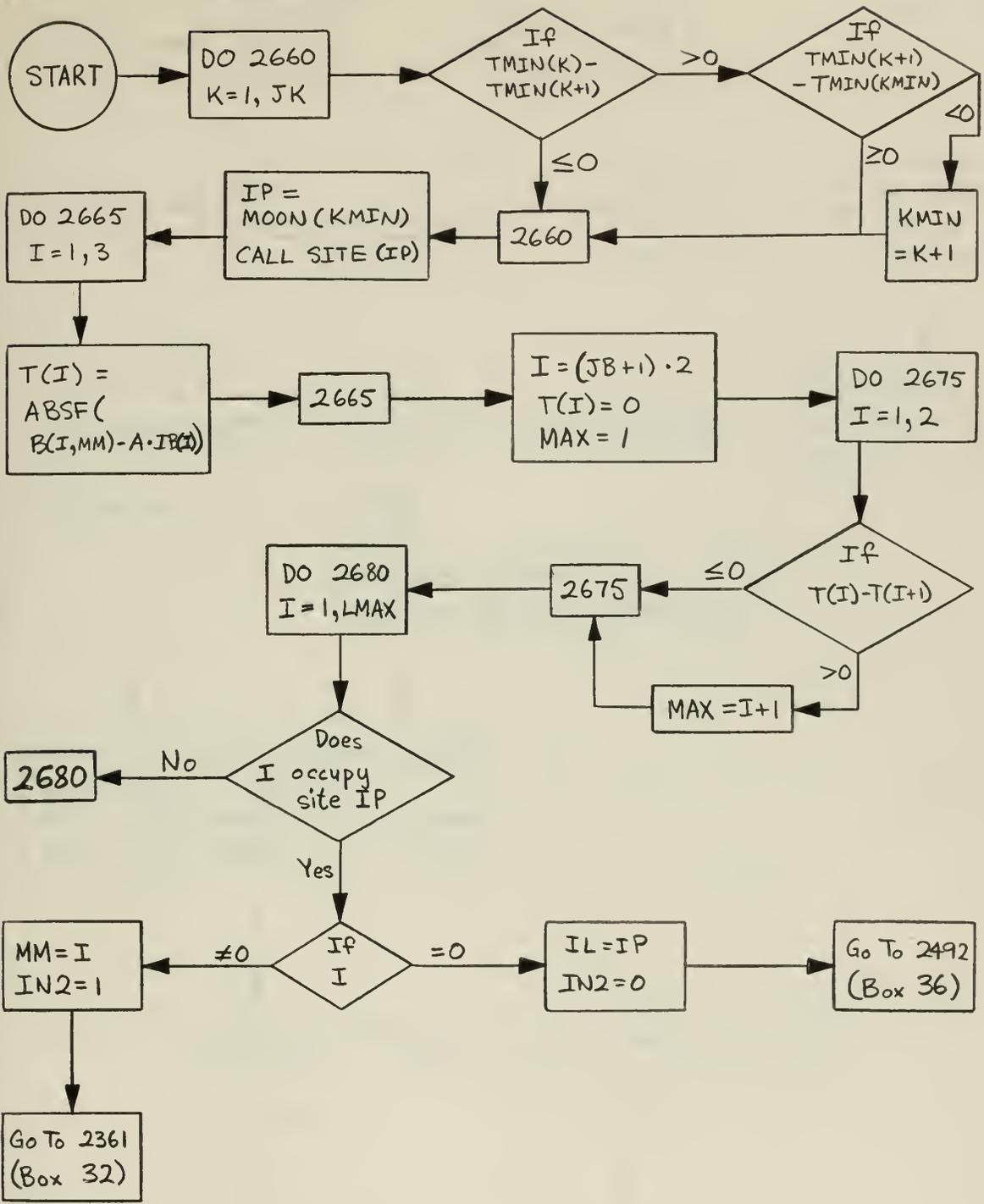




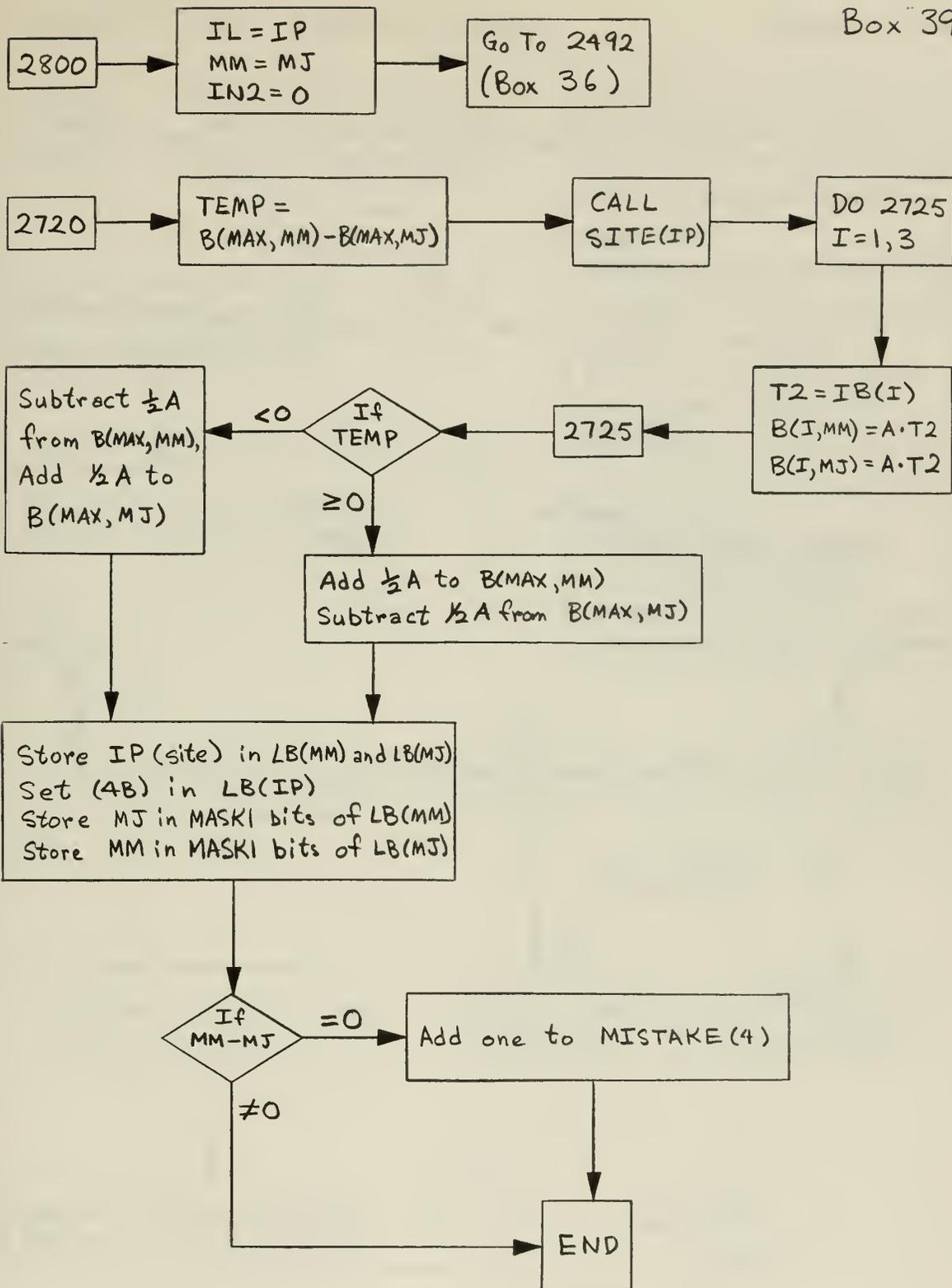


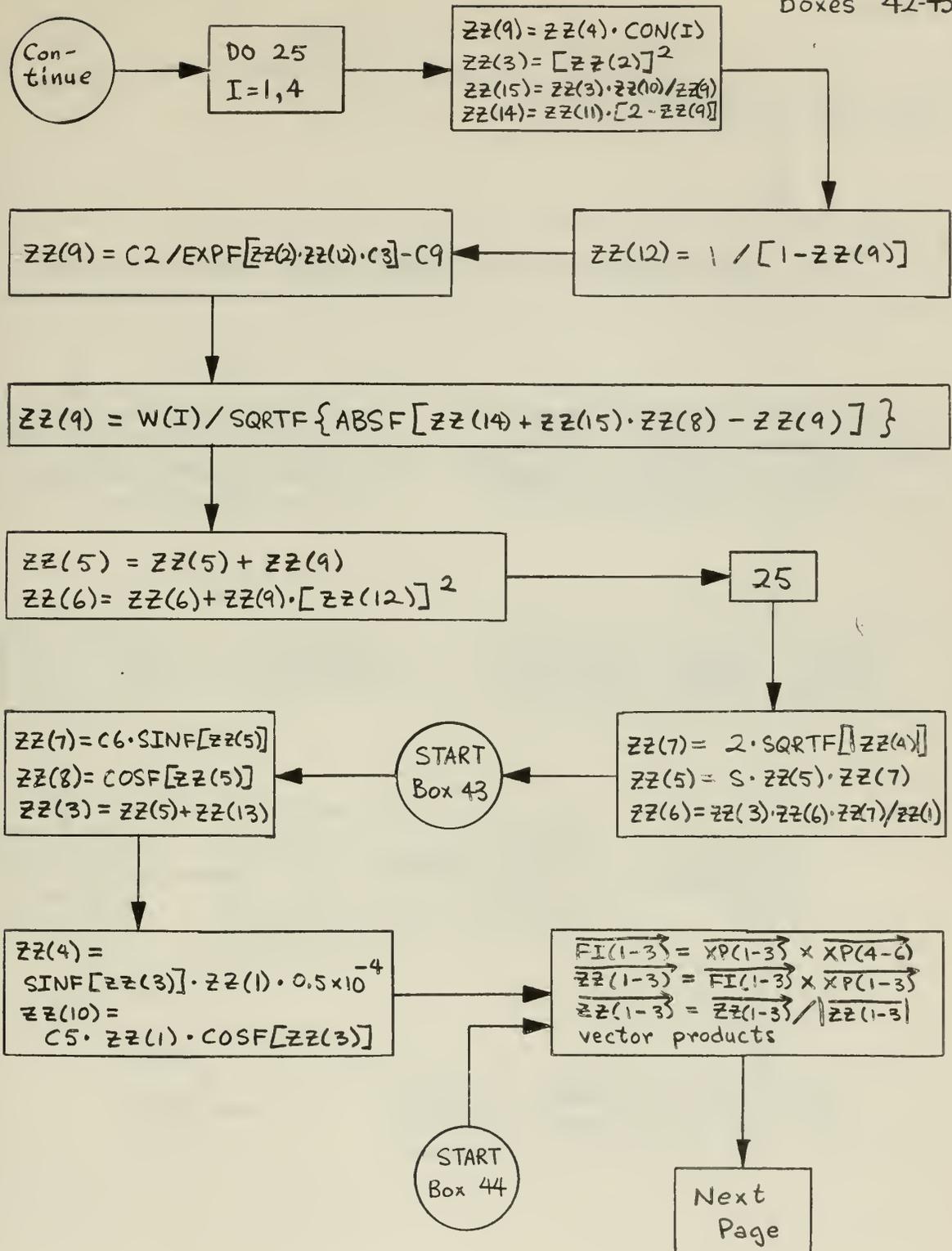
Box 39

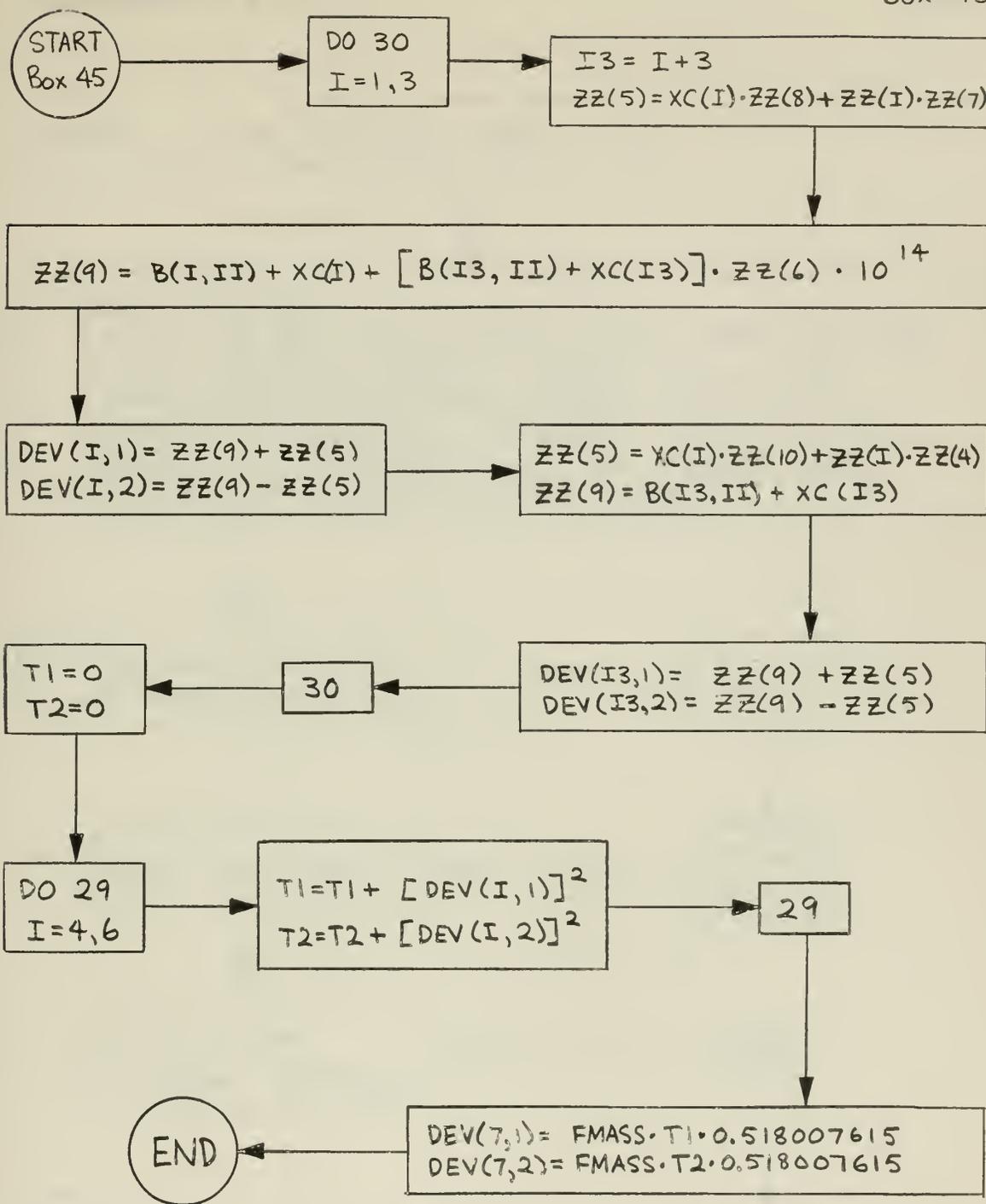


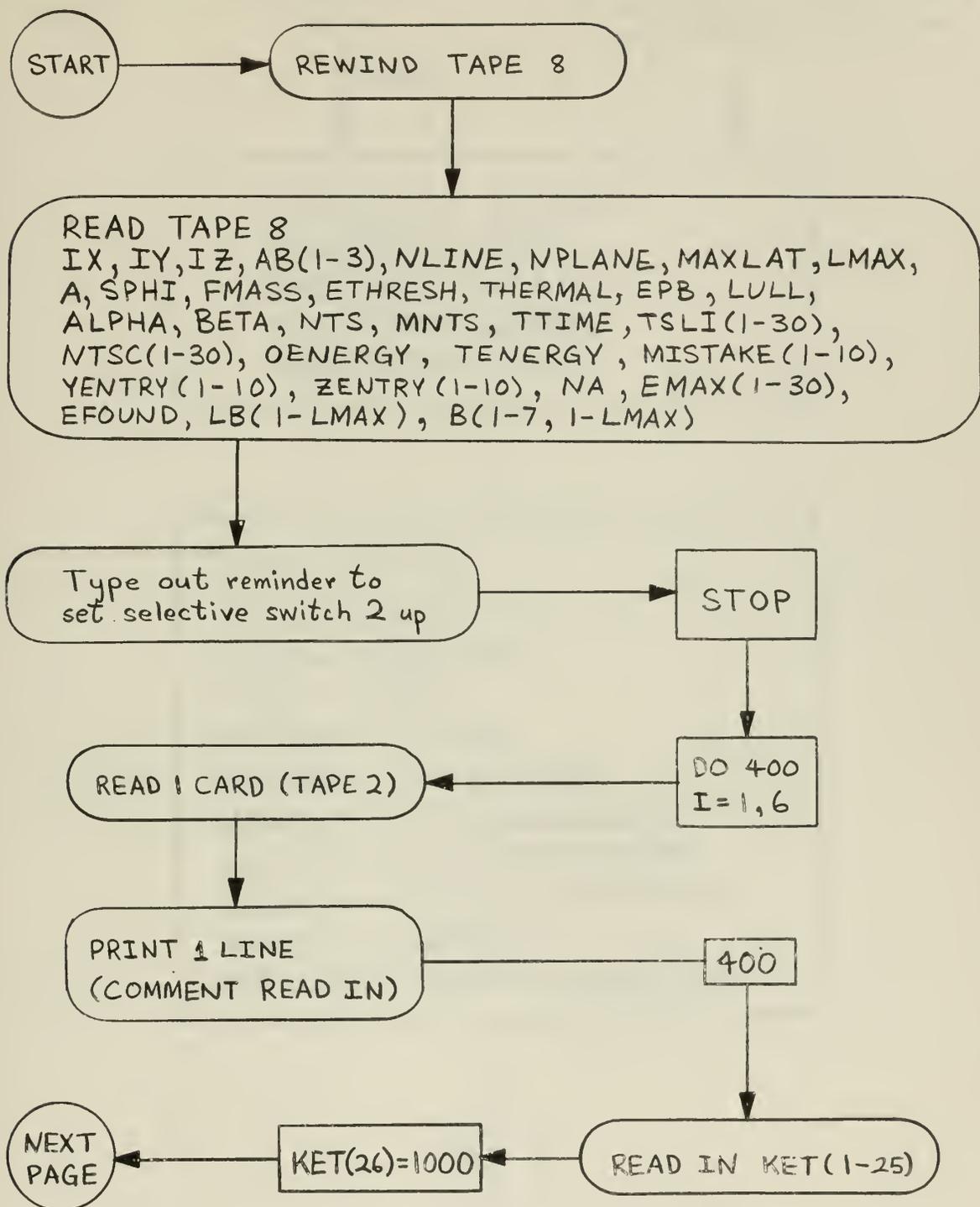


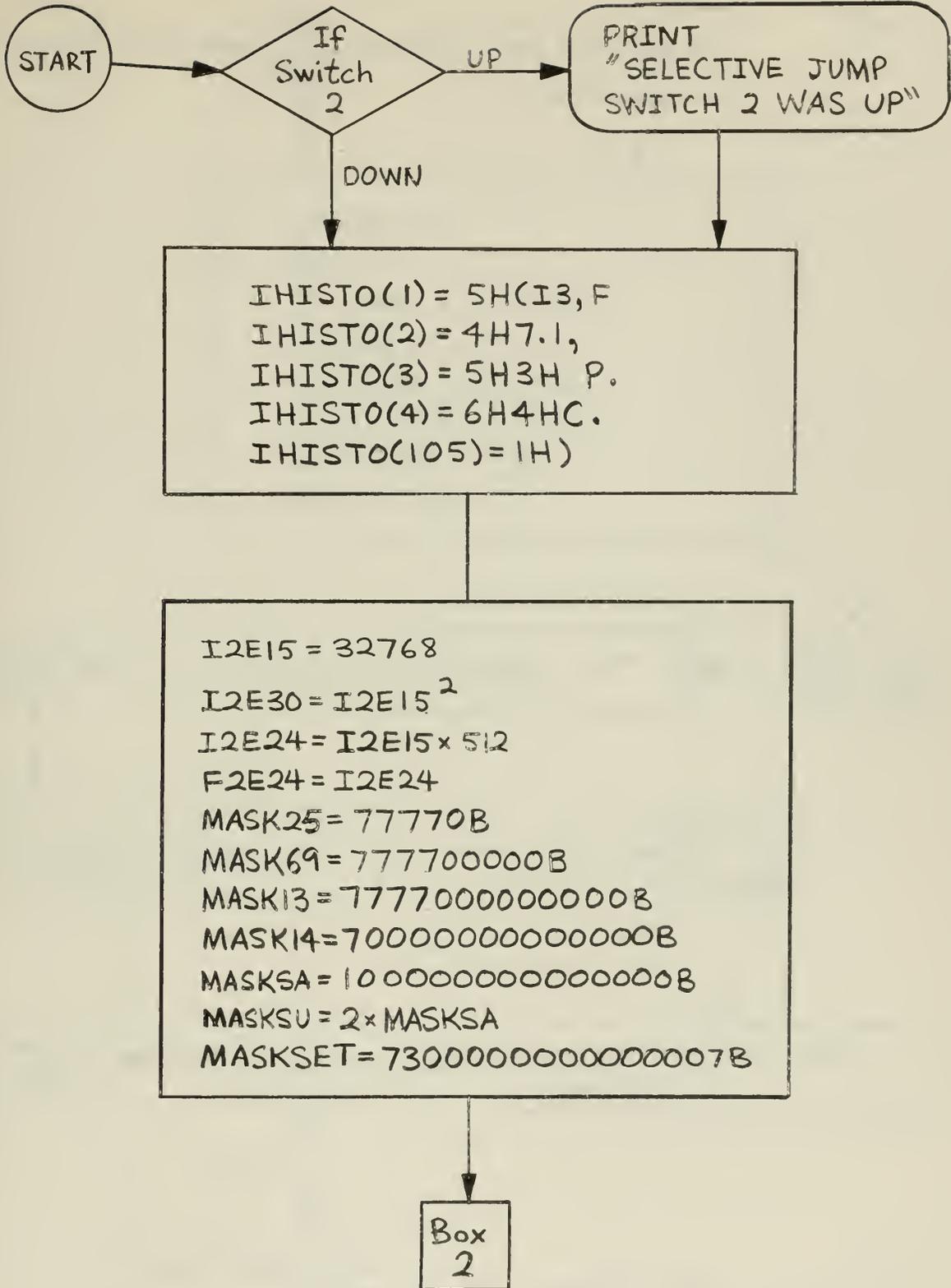
Go To
Box 39

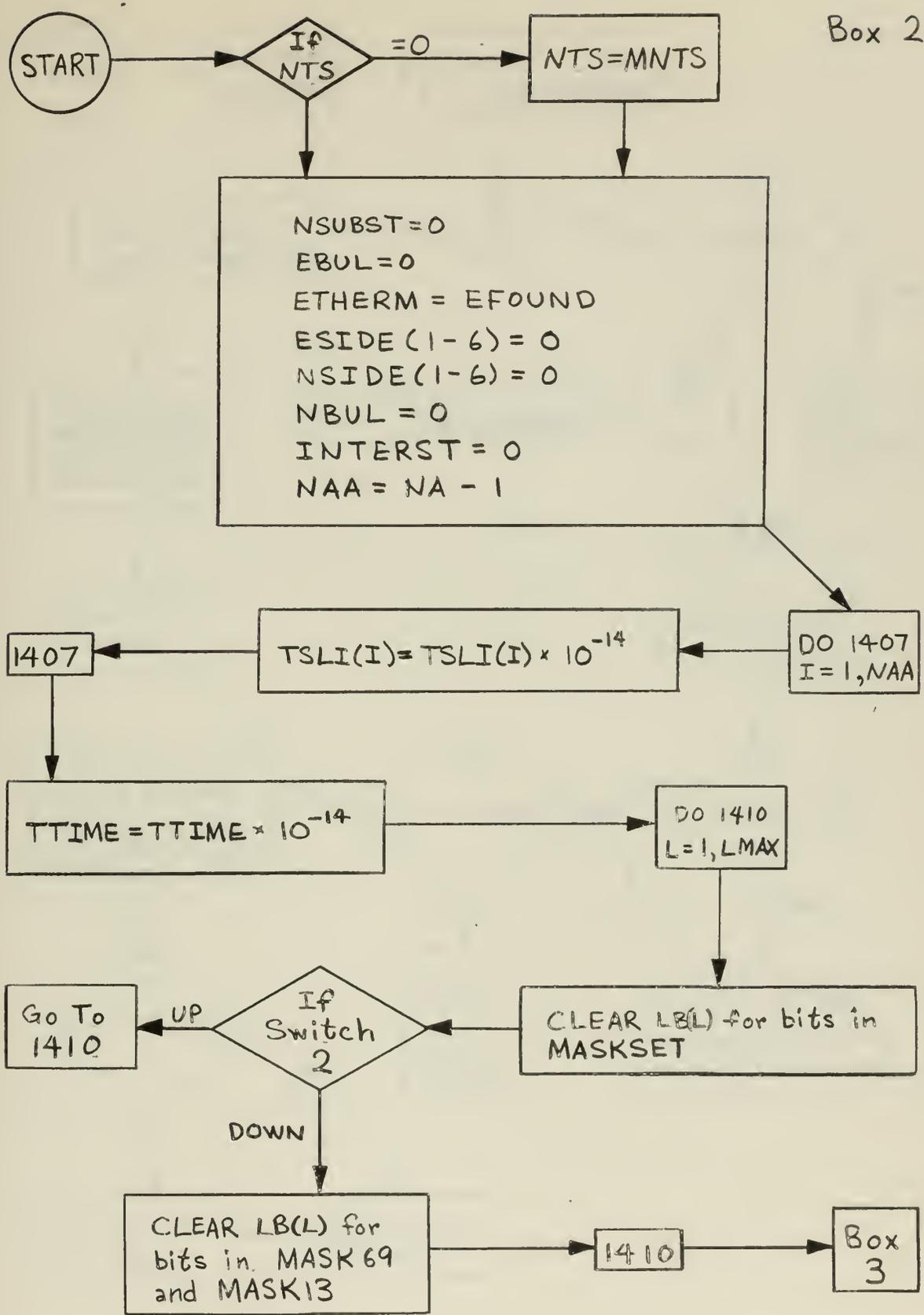


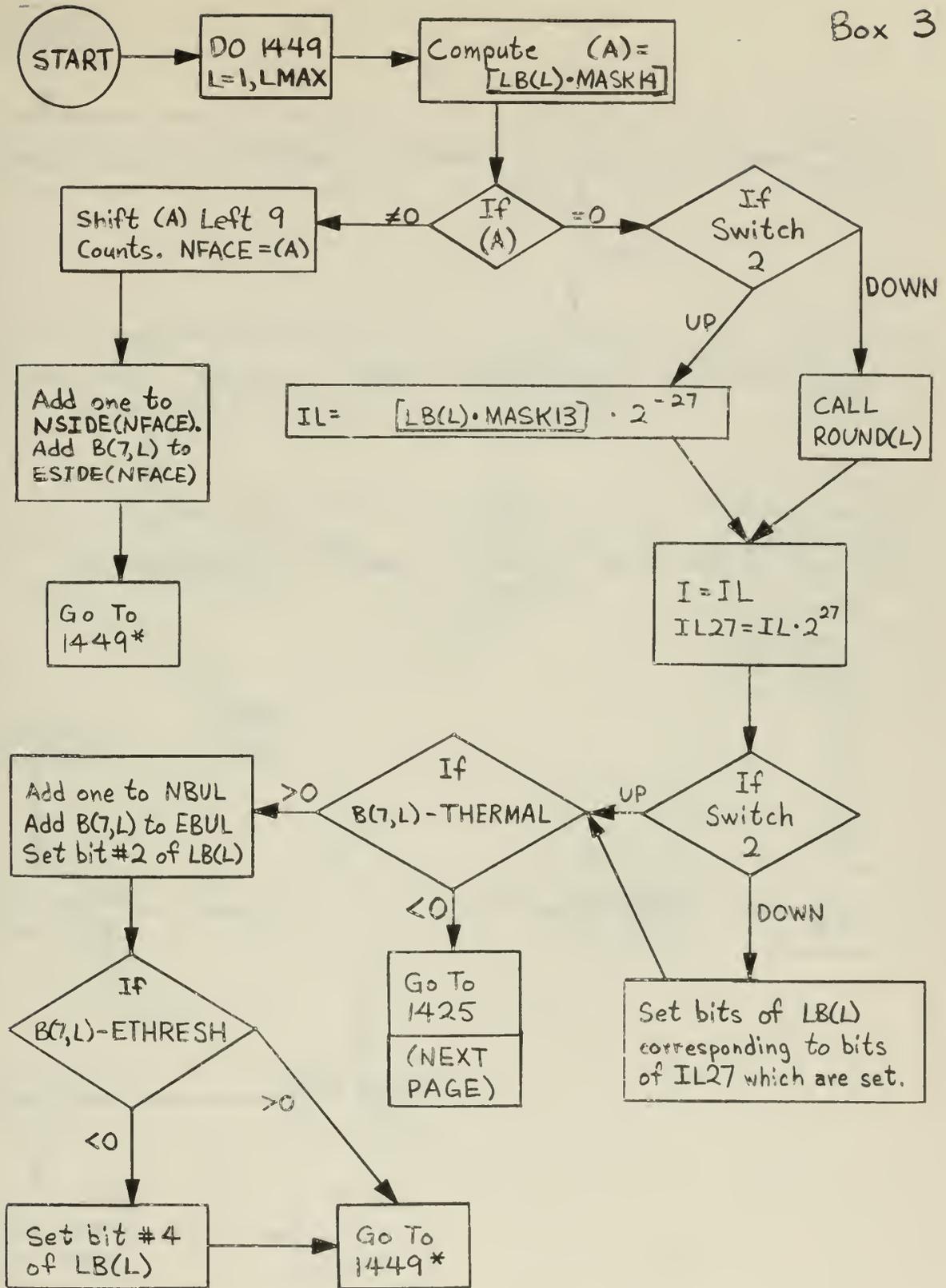




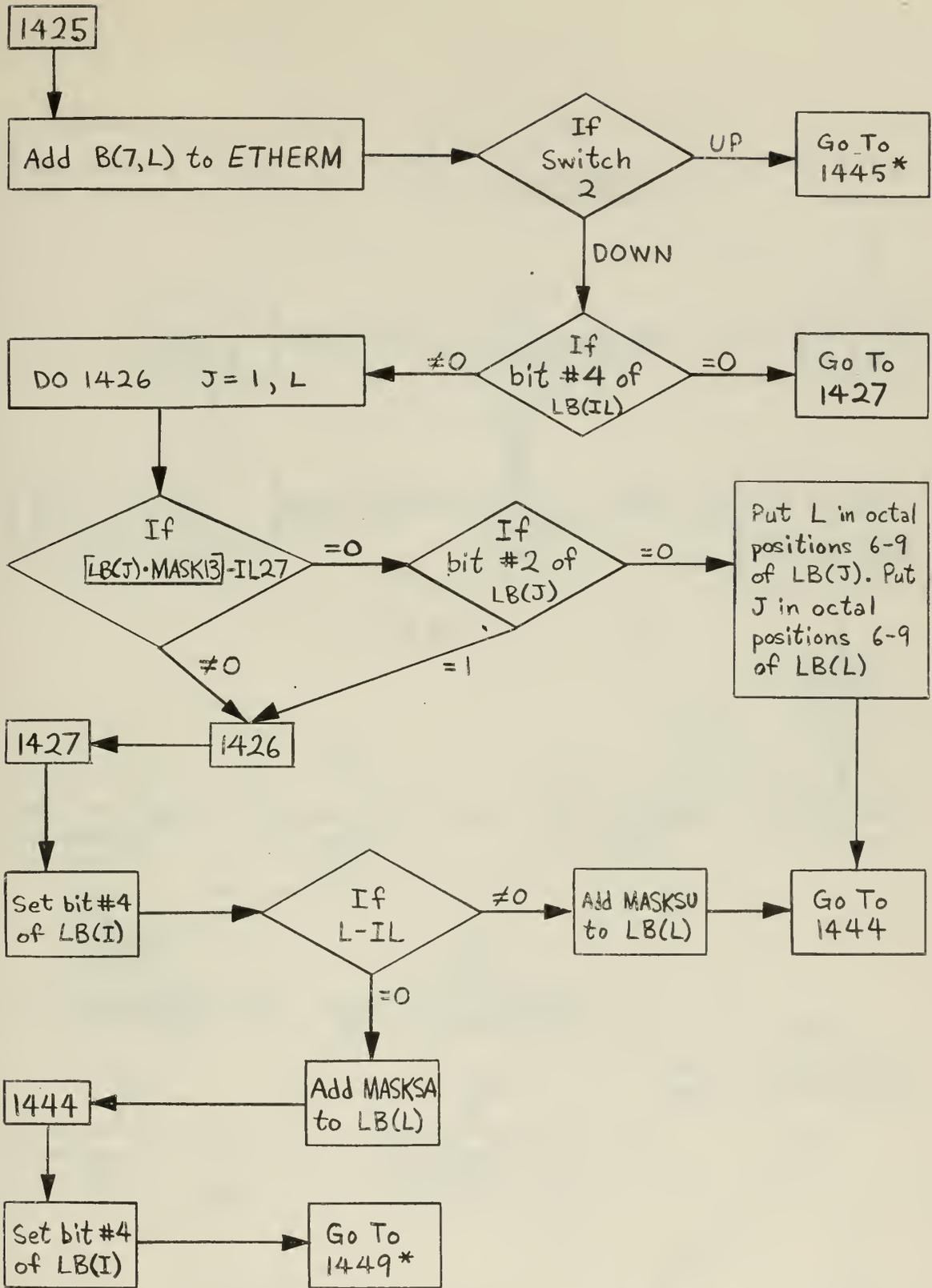




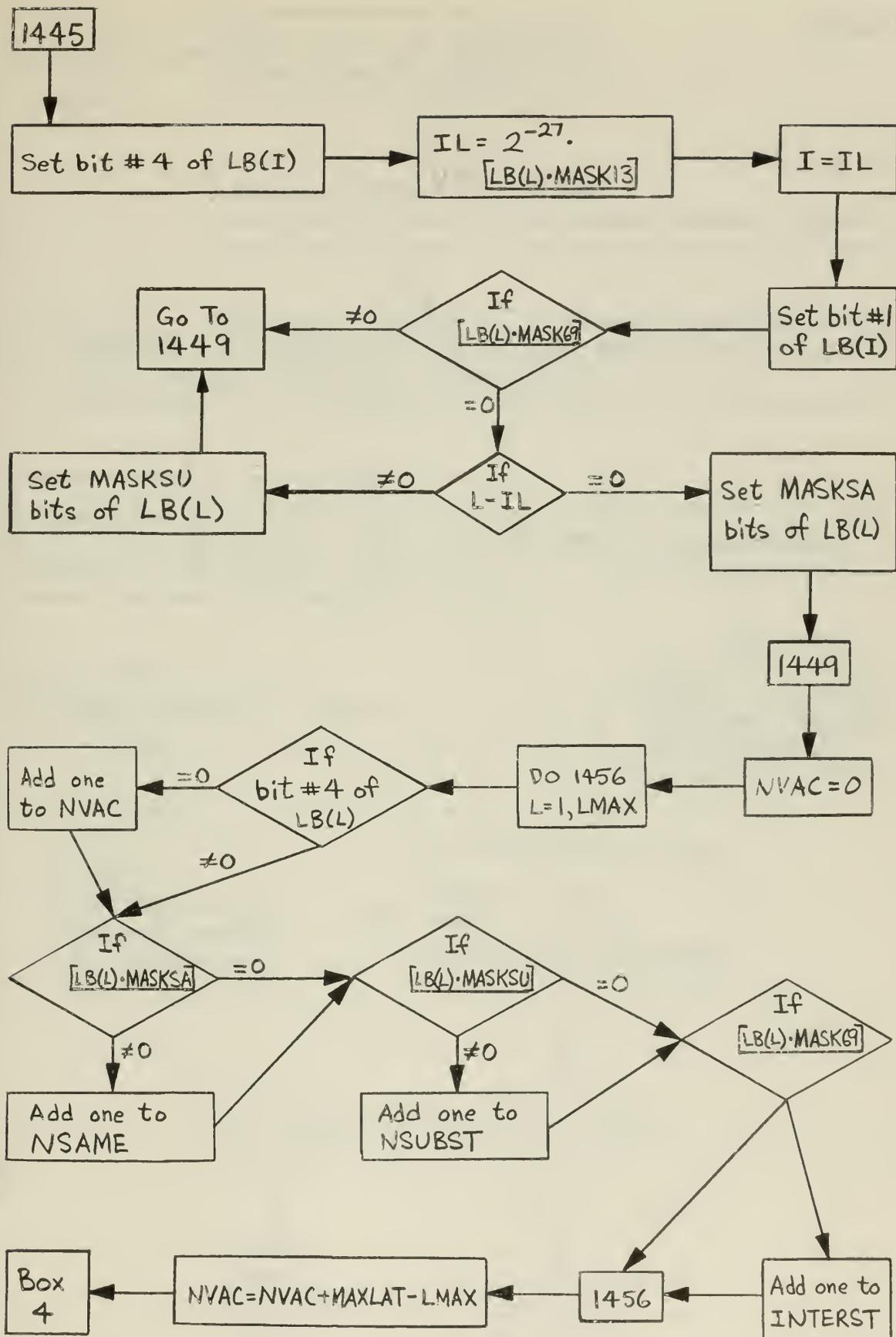


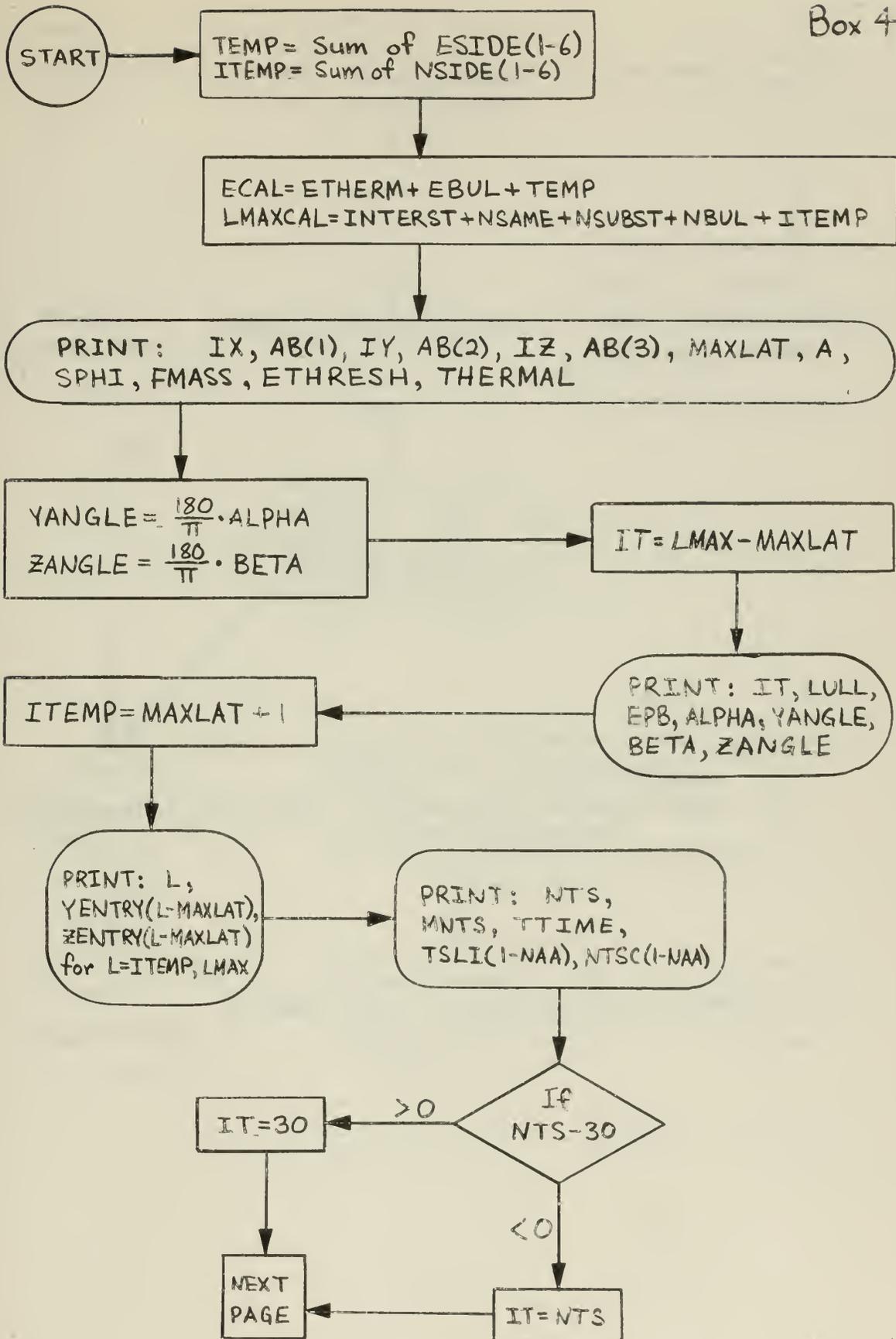


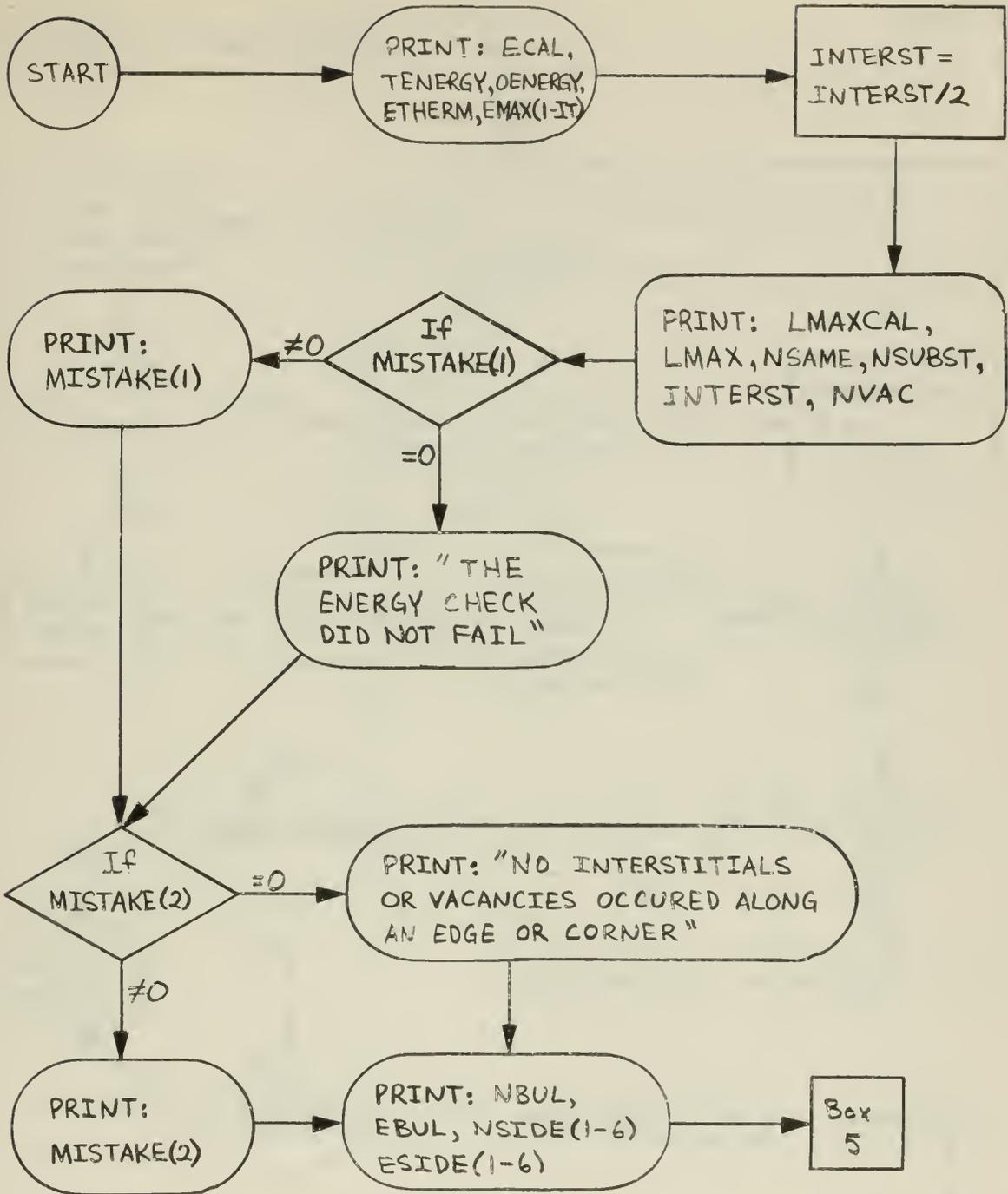
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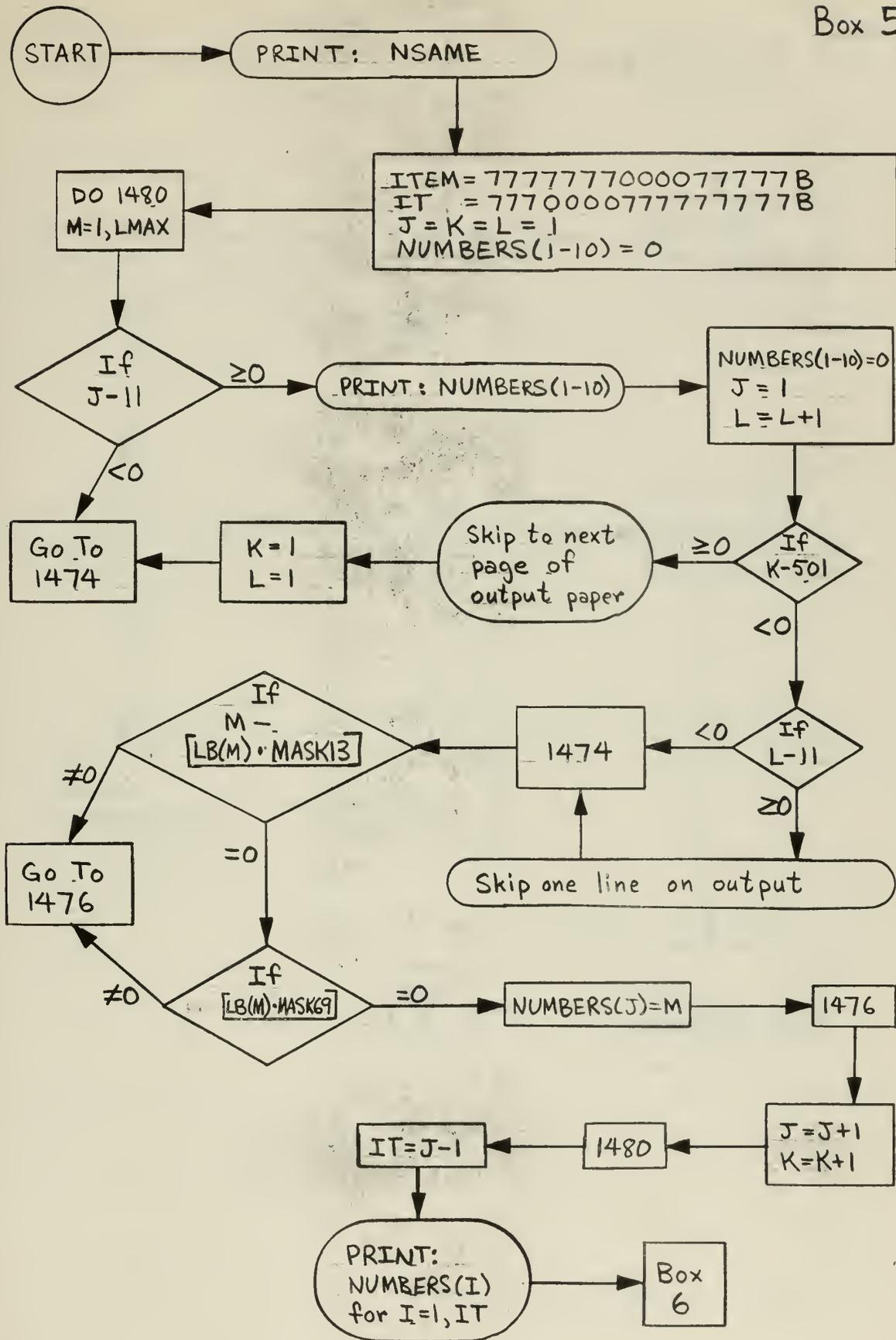


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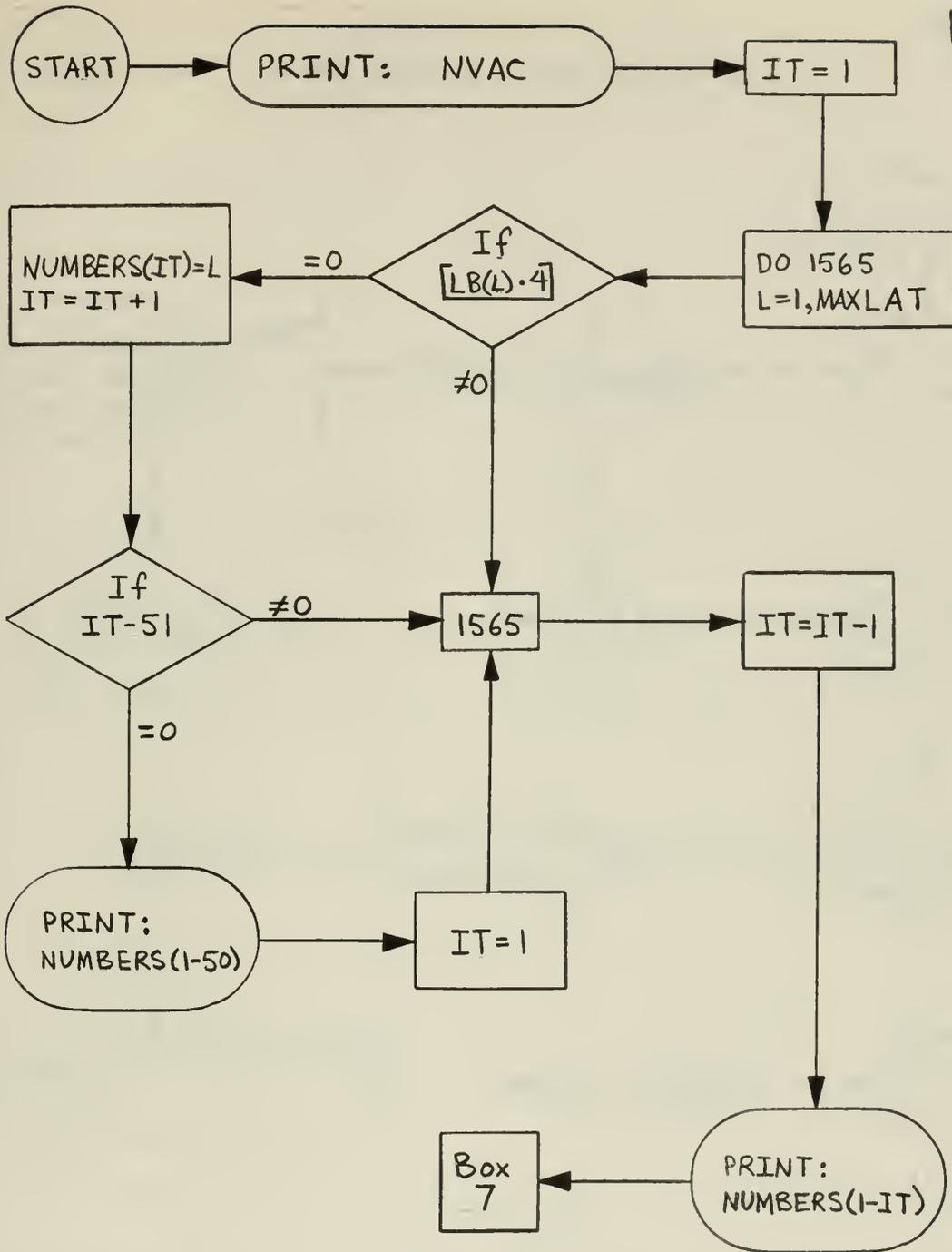


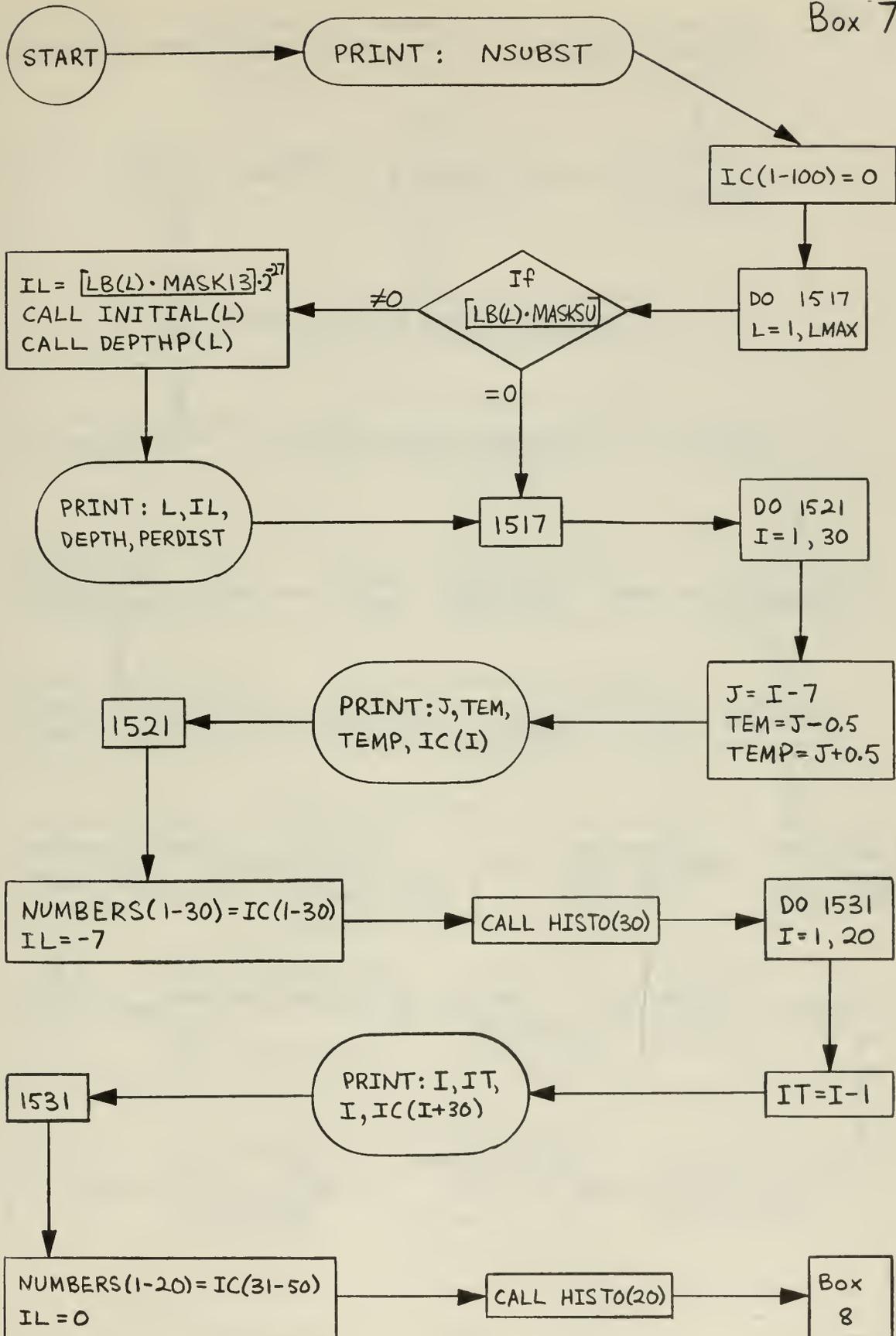


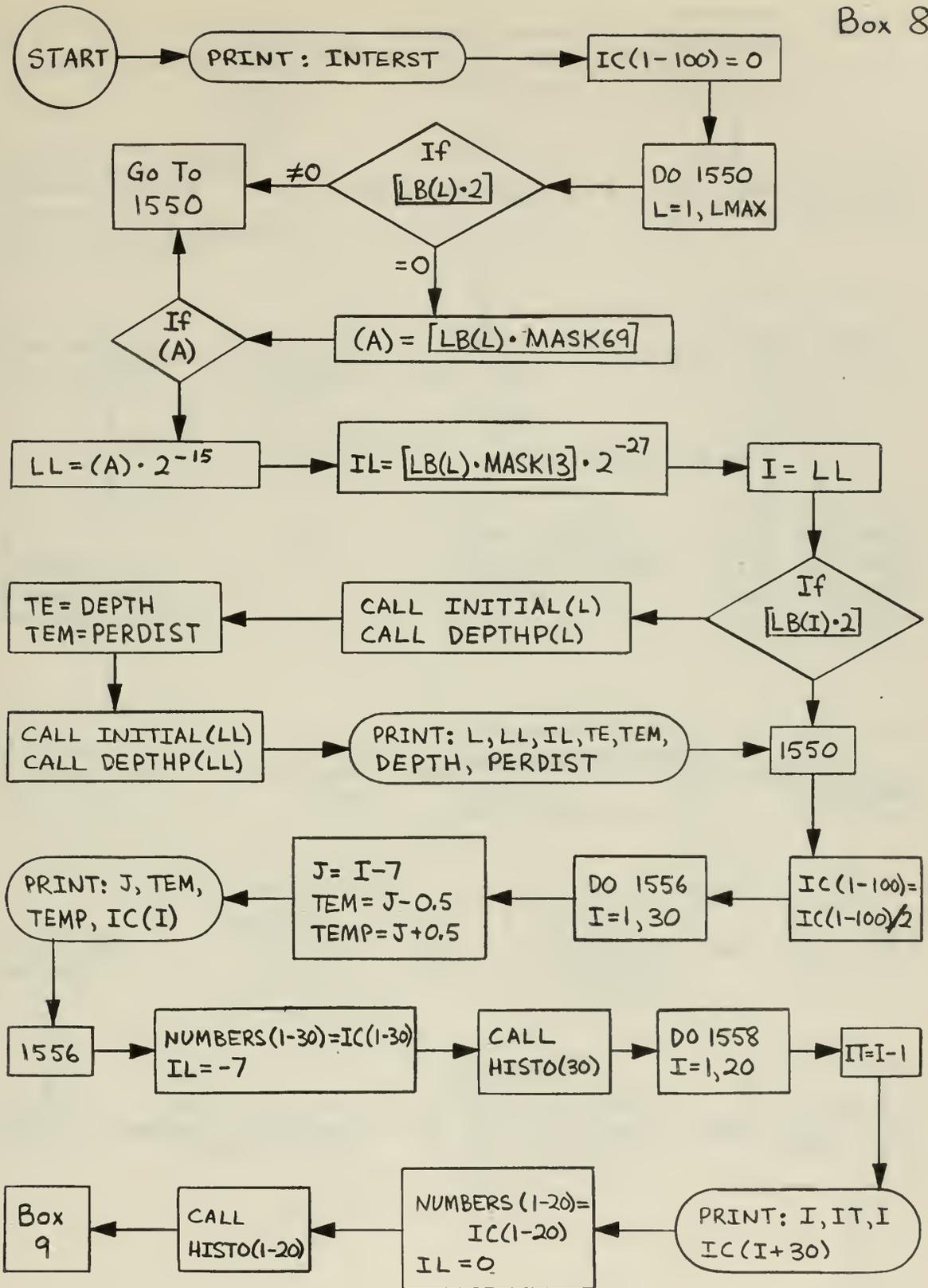


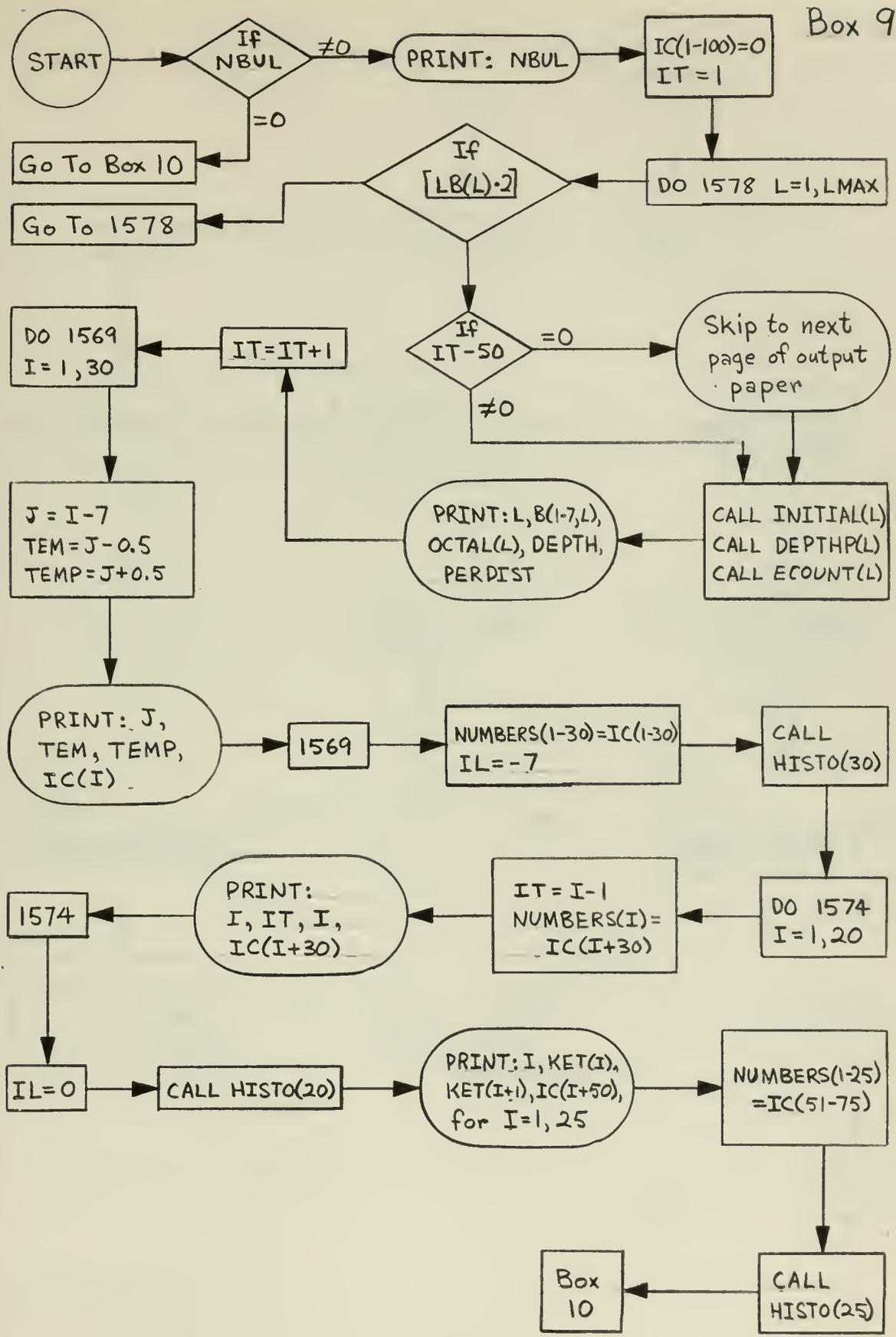


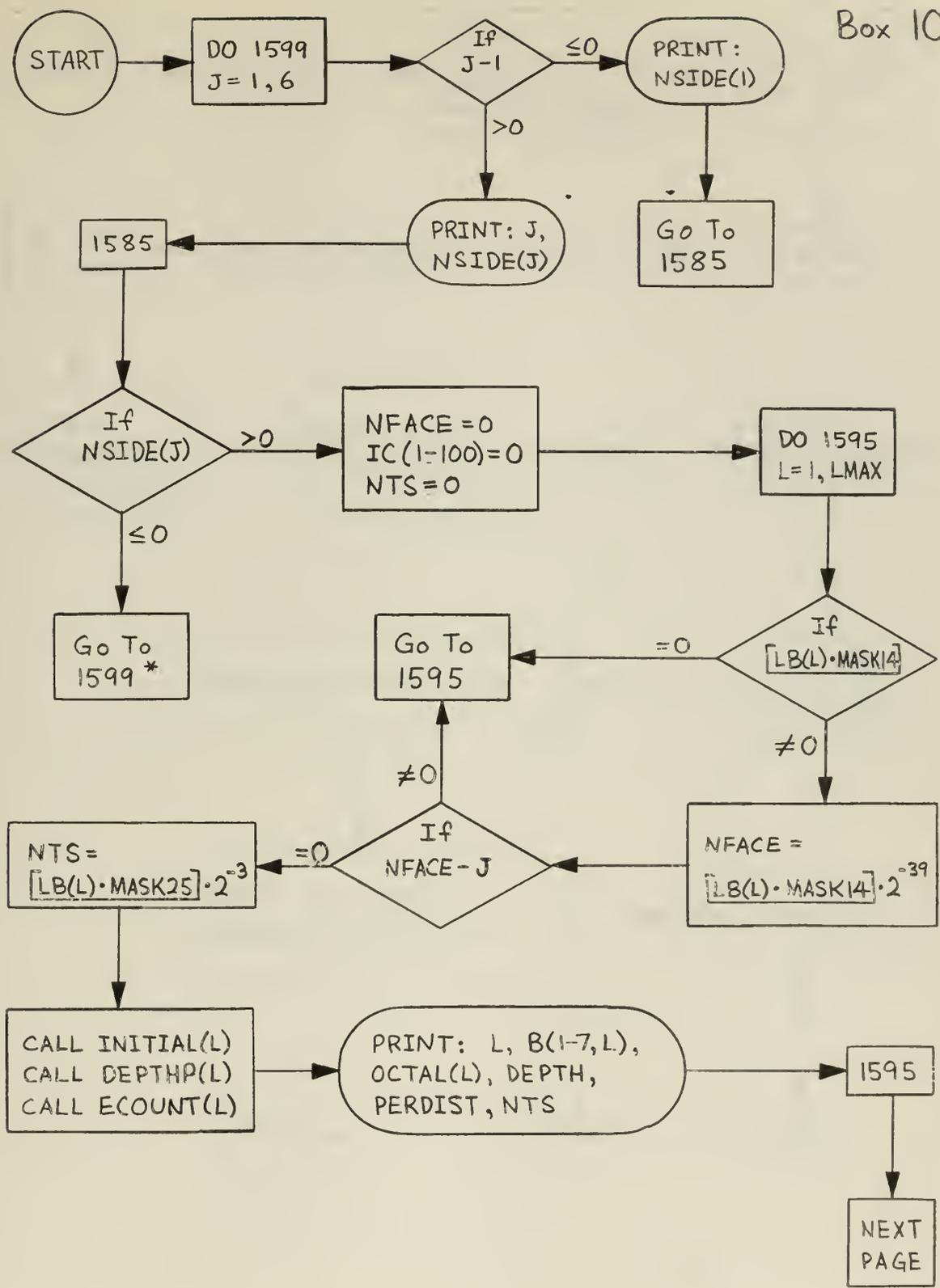
Box 6



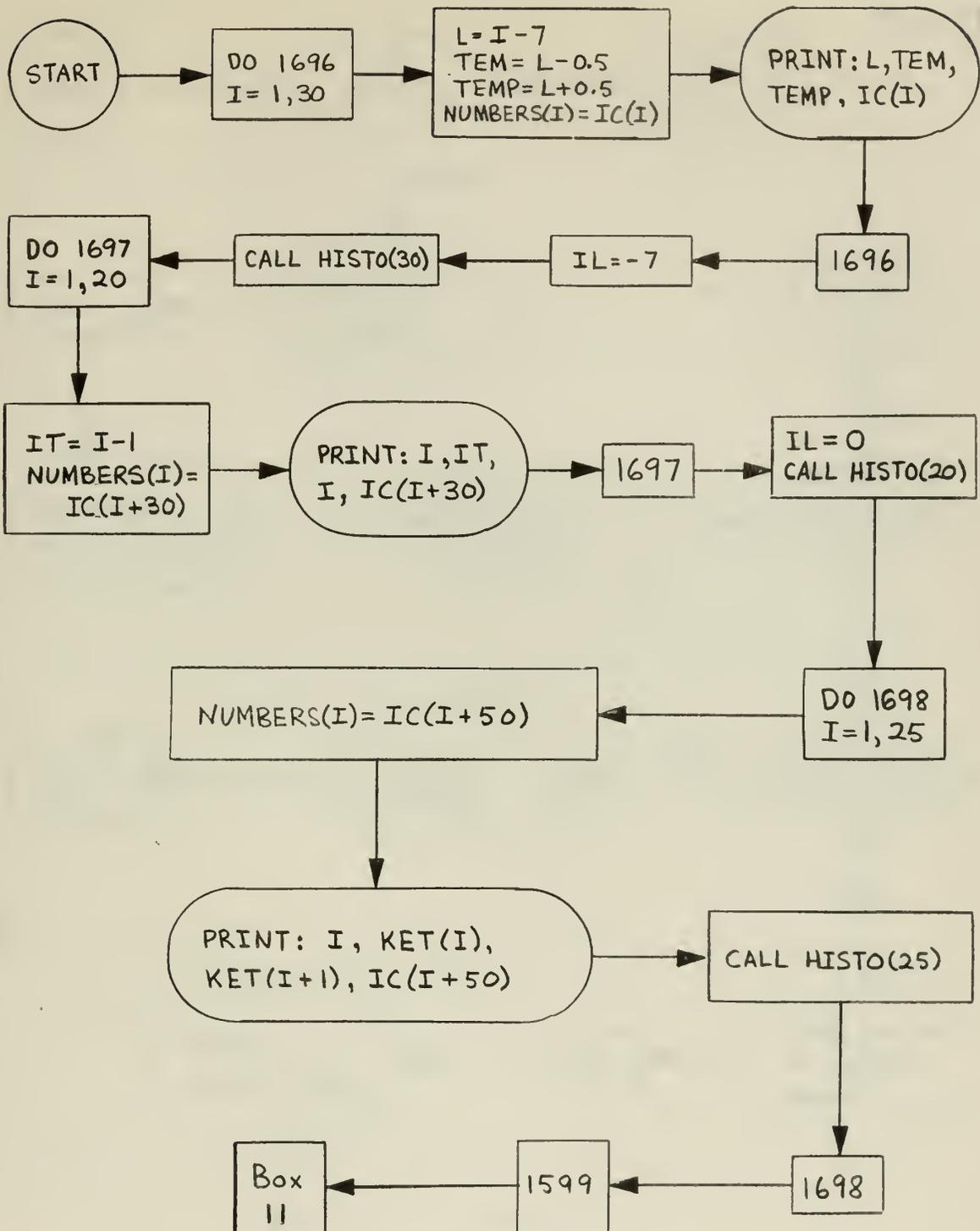


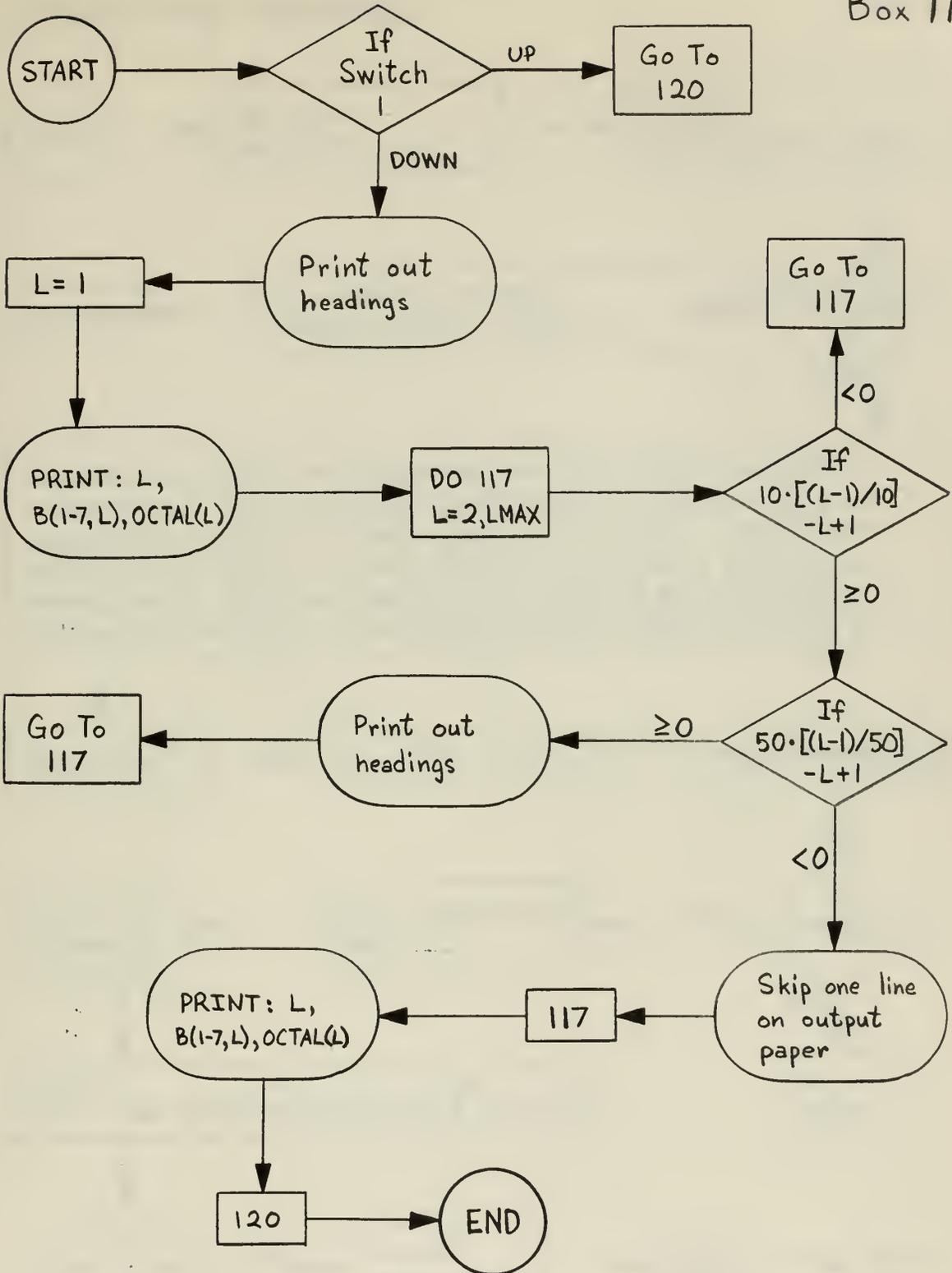


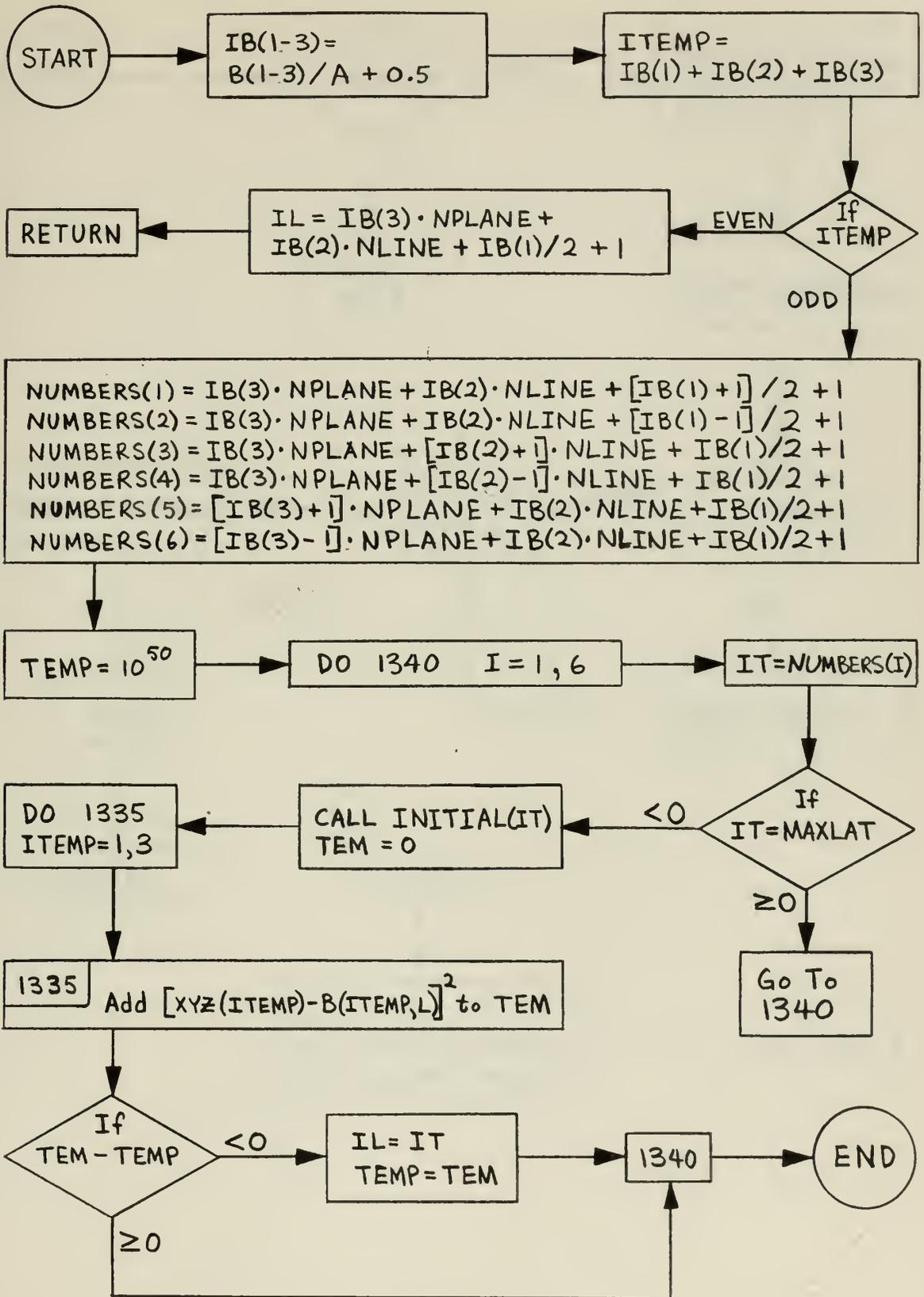


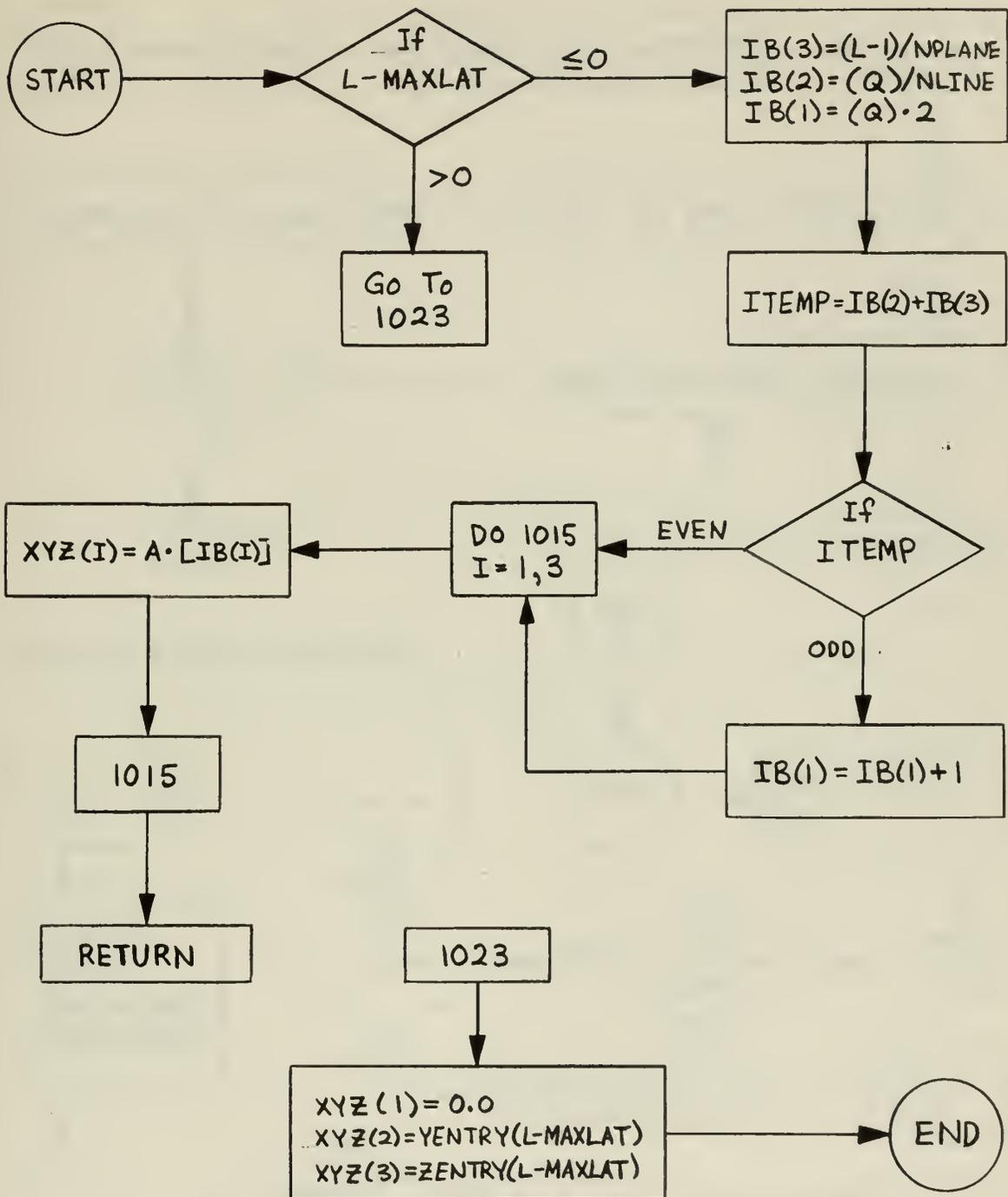


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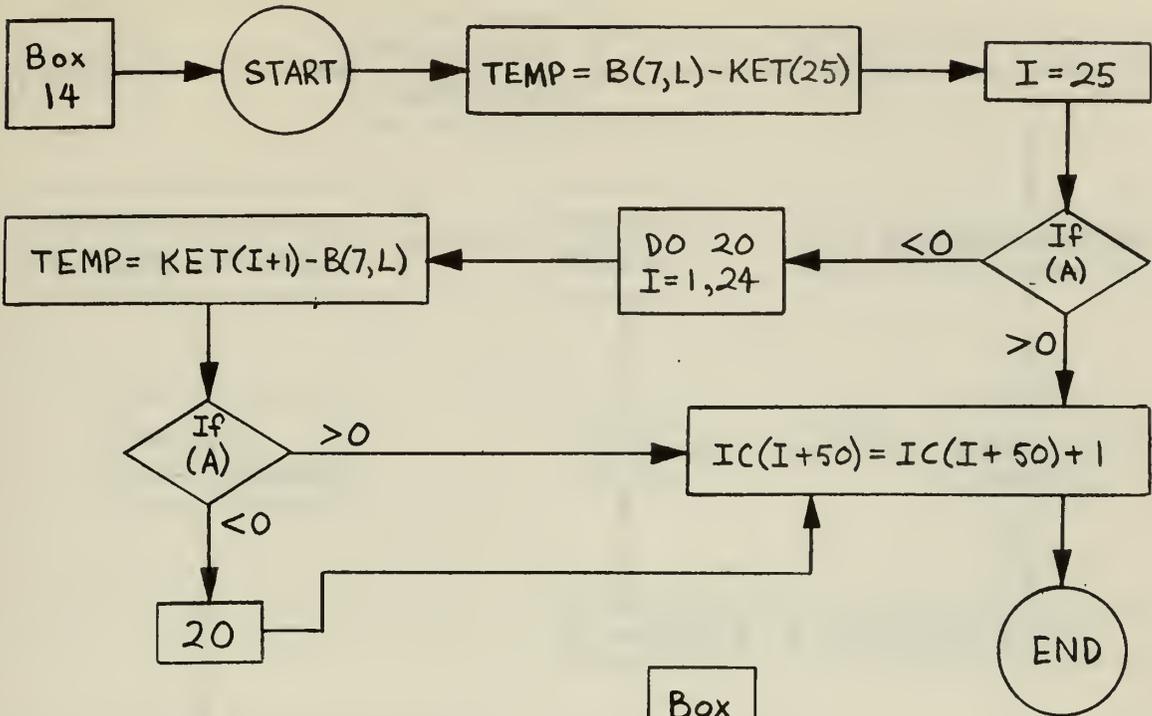




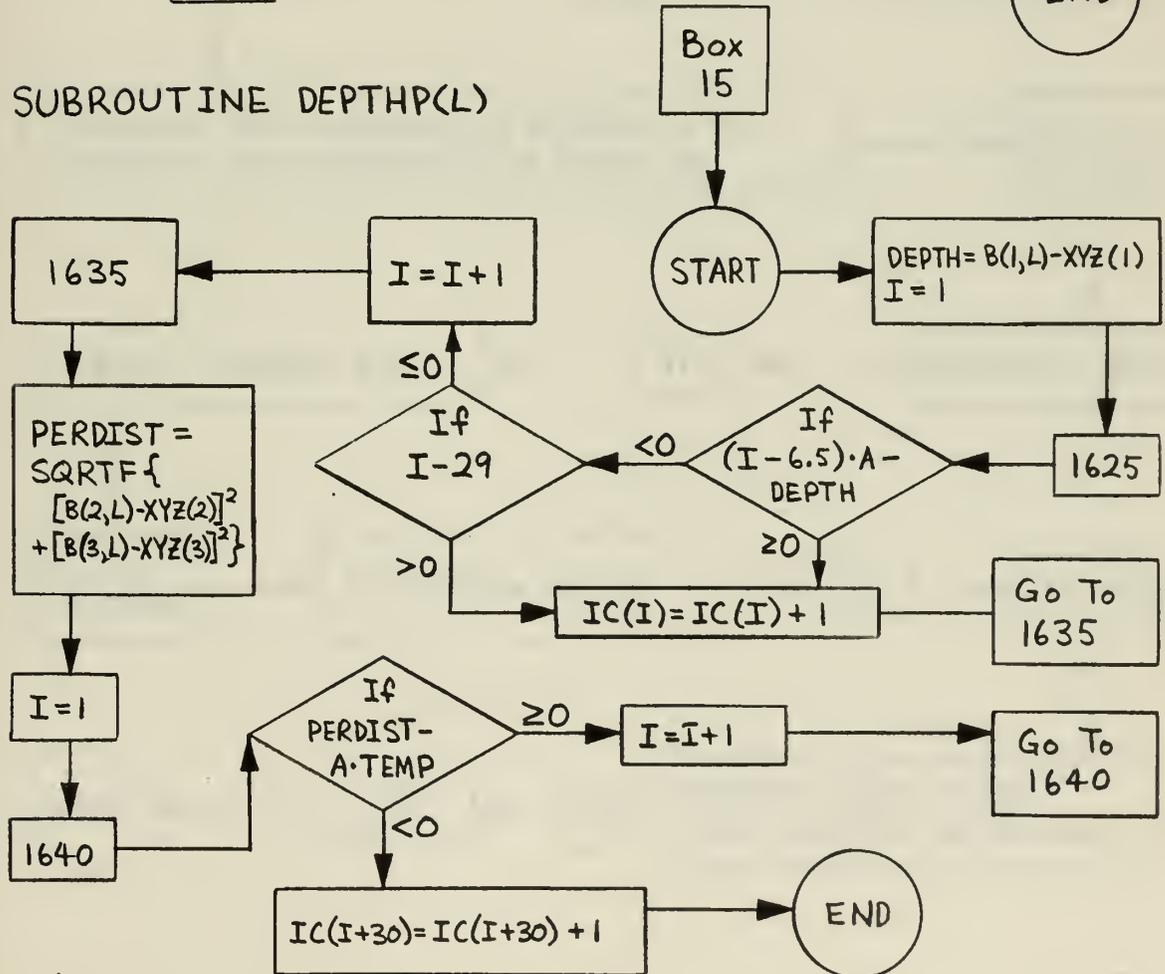


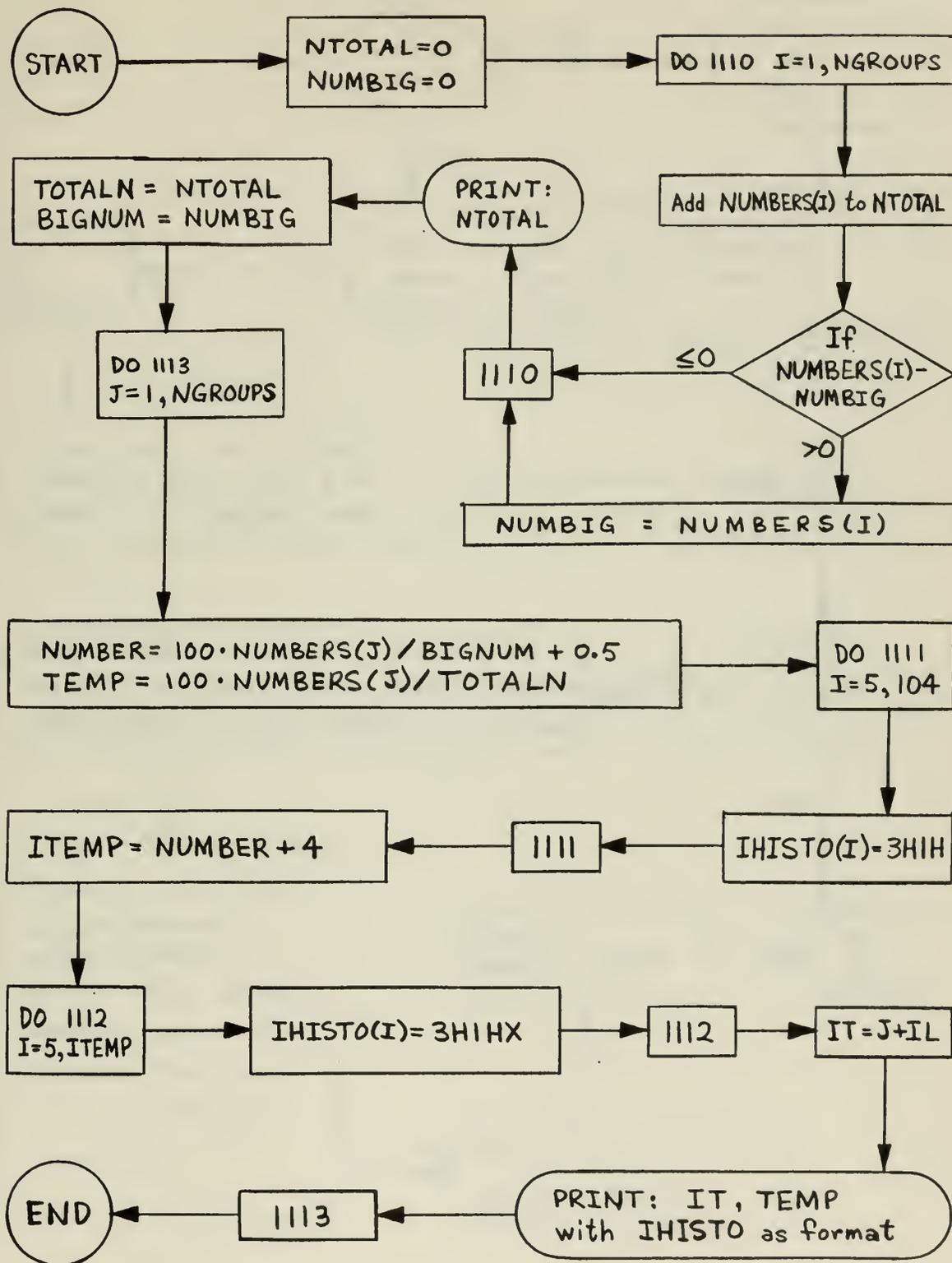
SUBROUTINE ECOUNT(L)

Boxes 14 and 15

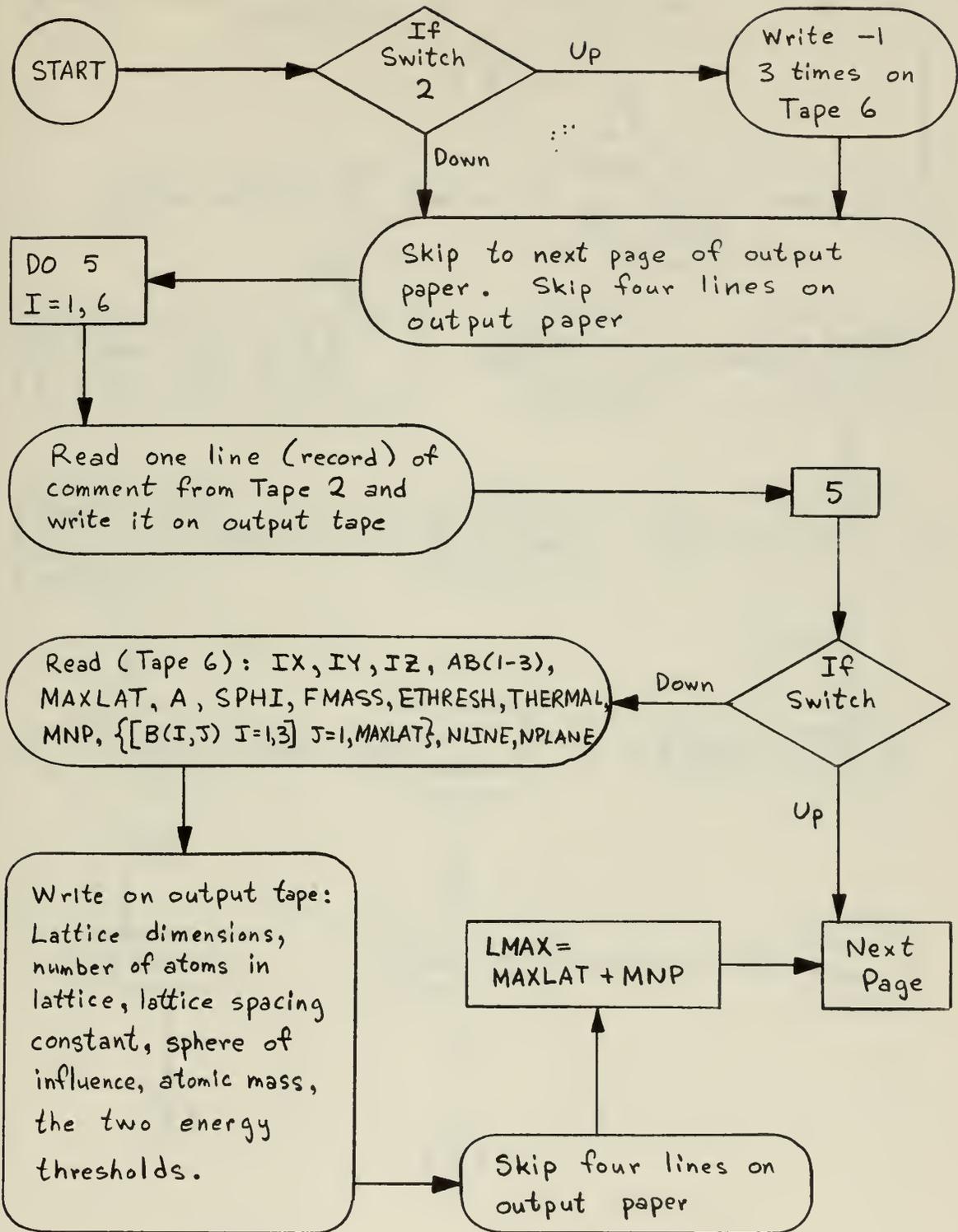


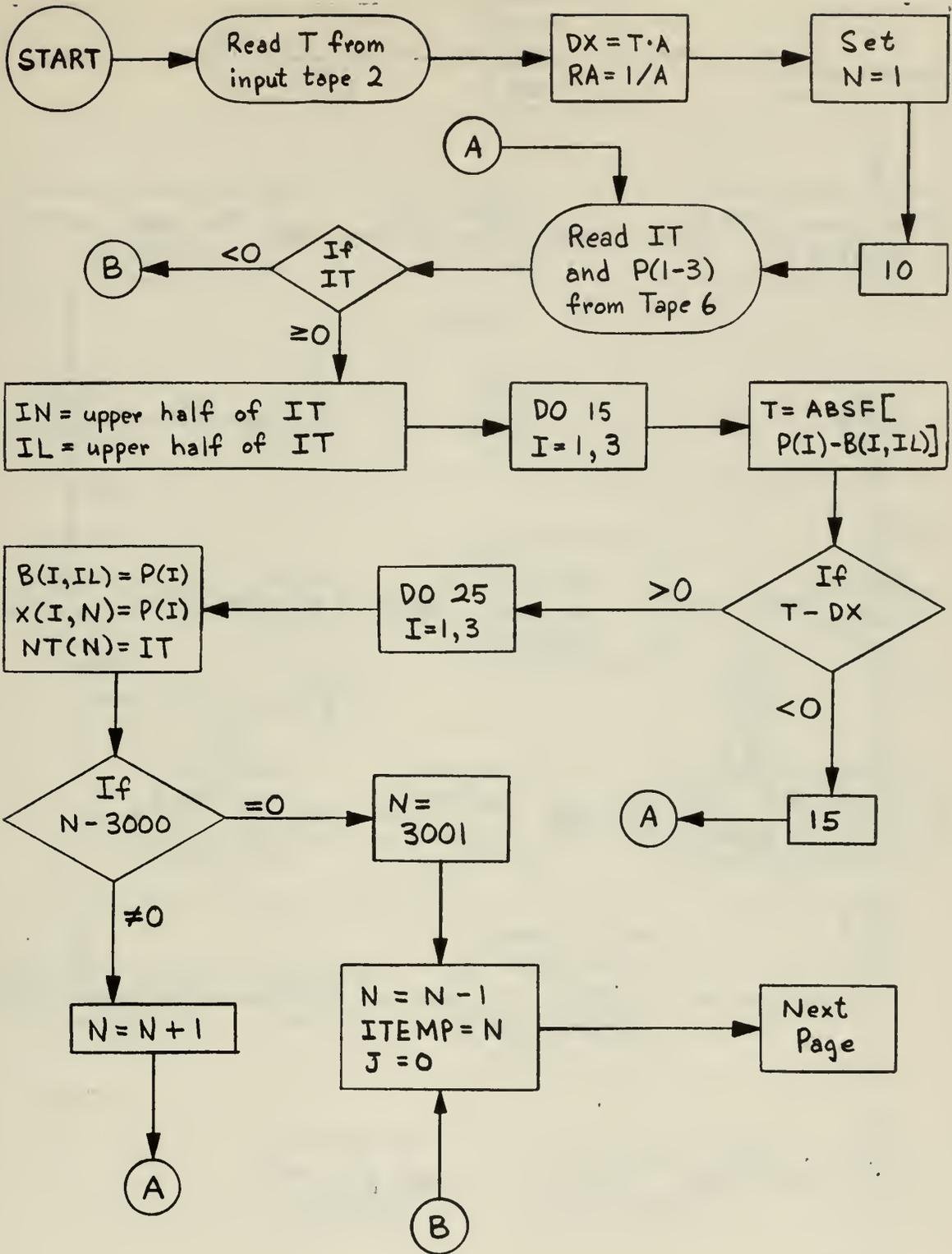
SUBROUTINE DEPTH(L)

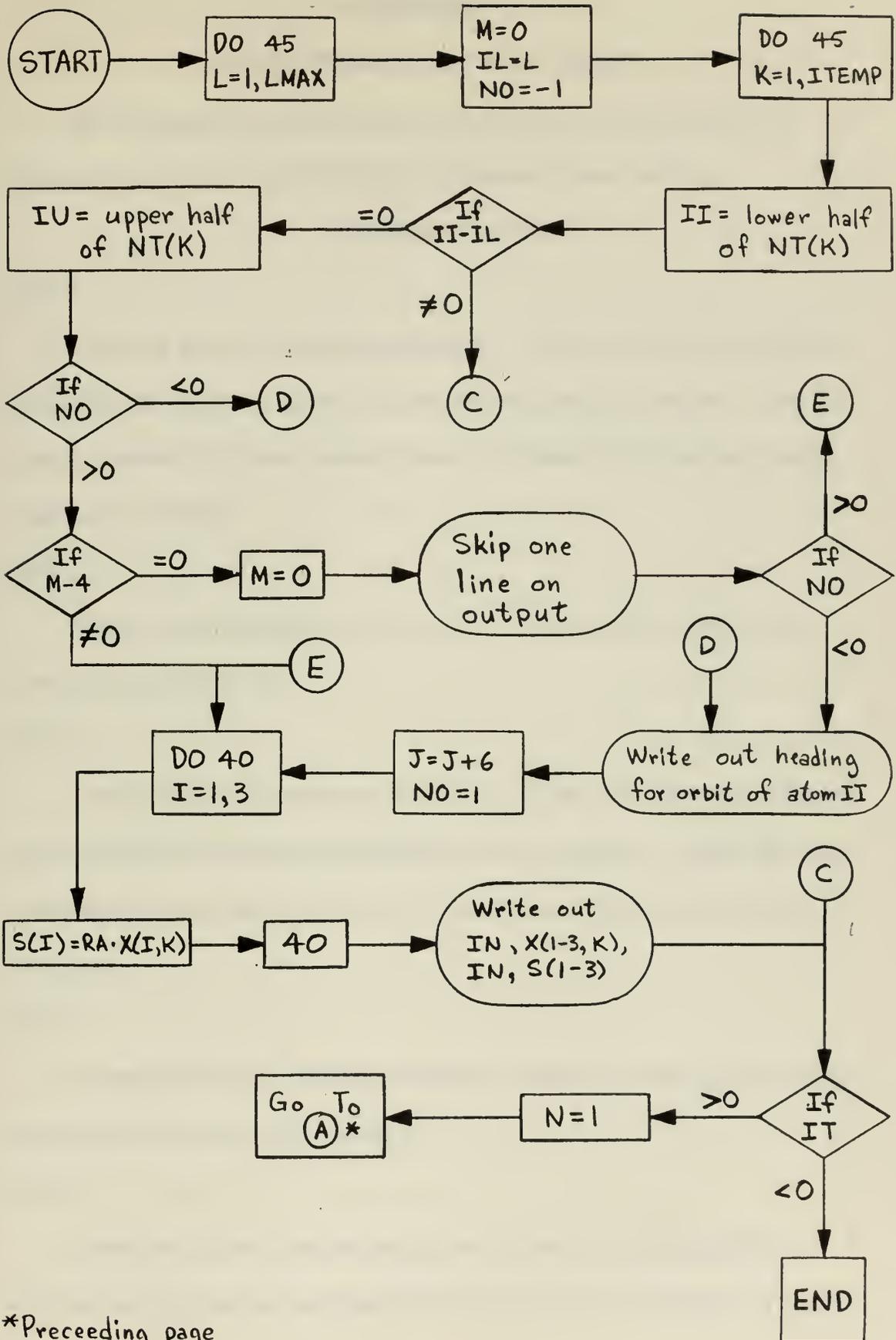




PROGRAM RON







*Preceding page

APPENDIX V

DESCRIPTION OF THE FLOW CHARTS

The explanation given below is to be used with APPENDIX III (Program Listings) and APPENDIX IV (Program Flow Charts).

PROGRAM MASTER

BOX 1

This box writes the title statement, "THIS IS PROGRAM MASTER" and as many comment cards (80 spaces per card) as desired. The DO loop is written for five comment cards at present, but can be readily changed if desired.

BOX 2

Reads input parameters for the run. Formats are given in the listing in APPENDIX III.

BOX 3

Changes lattice dimensions (IX, IY, IZ) into floating point format, and computes the physical dimensions of the lattice. These are then permanently found in AB (1-3). It must be kept in mind that IX must be ODD.

BOX 4

Computes NLINE, NPLANE, MAXLAT, LMAX (the initial LMAX) from the formulas given in APPENDIX II.

BOX 5

Computes initial lattice positions by use of subroutine SITE. Stores the site number and the fact that the site is occupied in the LB

array. Stores a -10.0 in each location of the TLAST array. This is necessary for collisions occurring in the first time step, otherwise these collisions would be ignored.

BOX 6

Writes initial lattice positions on Tape 6 in binary for eventual use by program RON. Also sets initial or zero values for the indicators shown.

BOXES 7, 8, and 9

Sets initial constant values, sets values of masks, and reads in the input parameters for the appropriate Born-Mayer potential, either potential 1, 2, or 3.

BOX 10

This box includes the regeneration process. Jump Switches 1 & 2 are raised, leaving Jump Switch 3 down. At the start of the next time step, the regeneration information will be written on Tape 7 in binary, and the tape will be rewound. To regenerate the run the program must be restarted, with all three jump switches in the raised position. After the program has started to read Tape 7 the jump switches may be reset. When the computer has finished reading Tape 7, the tape will be rewound. Further regeneration tapes may be made after this point has been reached. The main DO loop over the time steps is also started in this box. Immediately after the start of a time step the current values of TENERGY, N, IENERGY, and ENERGY are written on Tapes 3 & 4. The output on Tape 4 is usually transferred to the typewriter to provide

a visual check on the validity of the run as it progresses.

BOX 11

All decisions concerning continuation or abandonment of the run are made in this box. A jump can be made to the output section, the normal output dump made, and a return to this box, or abandonment, accomplished by the outside control of the jump switches. The run will be abandoned, after an output dump, if the most energetic particle has an energy less than THERMAL. However, the run will not be abandoned under this condition if other particles are to be shot into the lattice.

Additional particles will be shot into the lattice, if the proper jump switch is set, at the start of the next time step that is one less than a multiple of LULL. For example, if LULL is 3, and the proper switch is set in time step 6 (or 7), an additional particle will enter at the start of time step 8. The switch must be left in the set position until after the particle has been read into the program.

The input co-ordinates for the particle are given as - 1.0 for X, and the actual point on the front face of the lattice we desire to hit. The angles ALPHA & BETA are given, as is the energy. This box then calculates the proper co-ordinates and velocity components to achieve the desired impact point. Since the new particle is the most energetic in the lattice, the Time Step Length is also recalculated at this time.

BOX 12

Here, the TSL is recalculated if the number of the time step is an

even multiple of JPB, and the first 30 values are placed in the TSLI table for output reference.

BOX 13

This is the only energy check made during the run, done every time step. The total energy (obtained as a sum of the individual energies) is compared with the original energy (the total amount shot into the lattice), and if they differ by more than 1%, the MISTAKE (1) error indicator is increased by one.

BOX 14

The value of ENERGY is recorded in the EMAX table for the first 30 time steps, the total energy, TENERGY, is recalculated, and the LB array is reset and now shows that none of the atoms have been through the current time step.

BOX 15

The major DO loop on the particles is started here, with the LB array used to check certain conditions on each particle. If the atom:

- 1) Does not have an energy greater than THERMAL, or
 - 2) Has left the lattice, or
 - 3) Has completed this time step, or
 - 4) Has been through INVAC and has not had a collision since,
- a jump is made to the end of the DO loop, and the next atom is considered.

Therefore, only those atoms are considered that satisfy all the following conditions:

- 1) The atom is a bullet, i.e. has more energy than THERMAL,
- 2) The atom is in the lattice,
- 3) The atom has not completed this time step, and
- 4) The atom has not been through INVAC since its last collision.

If all the preceding conditions are satisfied, the initial values of the counters and lists shown in BOX 15, APPENDIX III are set to zero or other appropriate values. M, the fifth Index Register, is then set equal to L, the fourth Index Register. L, as such, is not used for the rest of the DO loop, until this pass through the DO loop is completed and a new L is chosen.

BOX 16

All atoms within a mathematical box with sides 3.02 (A) (centered at M) are placed on the NUM list here. Atoms are excluded if they have left the lattice or have been through the time step. If the list contains only one atom (M is placed first on the list), then a jump is made to BOX 25 where another value of M is chosen from the LAST list. With other atoms in the box, indicators IN3 and NFACE are set to zero.

BOX 17

For every atom on the NUM list, the following parameters are computed with respect to atom M:

- 1) The undeviated distance of closest approach between centers, called DSTANCE (),
- 2) The time of closest approach between centers, also undeviated, called TMIN (),

3) The time when the two atoms are separated by a distance of SPHI, called T (). This is the actual time a collision would occur.

The distance is given in Angstroms, with the time in jiffys, relative to the start of the current time step.

Various conditions are now imposed on these quantities to insure the validity of these presumed collisions. An atom must pass all the conditions to insure that a collision will take place. The conditions are:

1) $(\Delta V)^2 > 1.0 \times 10^{-6}$,

2) DISTANCE () \leq SPHI,

3) T () lies between \pm TSL of the start of this time step,

4) T () is less than 0.99999 TSL. This eliminates collisions that end too far into the next time step.

5) The TLAST for both atoms must be less than the absolute time of this collision.

If all of the above conditions are satisfied, IN3 is increased by one. If one or more of the conditions is not satisfied, T () is set equal to a large positive number (100 TSL serves this purpose in the program).

It should be noted that DISTANCE (4), TMIN (4), and T (4) are the parameters associated with the atom that is number 4 on the NUM list, i.e. NUM (4), and so on.

BOX 18

The minimum time on the T () list is found. All those on the NUM

list whose corresponding T's are equal to the minimum time, or within (CUTOFF)(TSL) of the minimum time are then placed on the KHIT list. Atom M is placed first on the KHIT list. At this point, if INPUT is zero, the KHIT list is duplicated on the LAST list. This occurs only when M equals L. INPUT is increased and the next box is entered if there is more than one atom on the KHIT list, i.e. another atom besides M. If there are no other atoms on the KHIT list, a jump is made to BOX 25, and M is set equal to the next atom on the LAST list.

BOX 19

This box and the next are concerned with the two body interaction itself, and the subsequent scaling methods for energy and velocity. These scaling methods are used whenever M collides with more than one atom. The pre-interaction velocities and energies are stored in the SAVE array. The COLD list is set to zero, and J is set to KHIT (JA). JA is the index used for the KHIT list in this box, M then hits the atoms in order of their placement on the KHIT list. JA is initially two, and increases up to and including NMAX.

With J selected, LB (J) is checked, and if J is a member of an interstitial pair, NPAIR is set to 3. The indicator NPAIR is used in BOX 24 to insure that the appropriate action is taken with respect to J's interstitial partner after the collision is over.

Since the atoms on the NUM and KHIT lists do not have the same placement, a search is now made to find J on the NUM list. When this is done, we have the collision time, T, and the collision parameter, PAR.

The two atoms, M & J, are then moved ahead in time to time T. If M has already had one or more collisions, it must be moved back in time to the start of this time step, and then ahead to the start of this collision.

The interaction subroutine is then called. Outputs are contained in the DEV array as the new positions, velocities, and energies of M & J.

TLAST is now calculated for J, and J's co-ordinates and velocities are set to those of the DEV array. Notice that the TLAST for J does not include any portion of the time necessary for the collision. If a portion of this time were included, significant collisions would be eliminated. The COLD array (1-6) contains the sum of the final position and velocity co-ordinates for M as given by the subroutine for all of M's collisions. The total energy lost by M (ELOST) then equals the energy gained by this J plus that gained by the other J's on the KHIT list. NHIT shows the actual number of atoms that have collided with M.

BOX 20

In this box, the scaling, by various means, of the velocities and energies of the atoms on the KHIT list is accomplished.

The temporary quantity T2 is set equal to the previous energy of M minus the amount lost by M in all its collisions.

If T2 is zero or negative, the energy and velocities of M are set to zero. With T2 negative, the energies and velocities of all others on the KHIT list must be scaled to conserve energy. All atoms are scaled in the same proportion, the absolute direction of their velocity vectors is preserved, their energies being scaled by the square of

the scale factor used on the velocity components .

In all cases , the spatial co-ordinates of M after the collision must be found . These are set equal to the numerical average of M's positions as computed by the subroutine . This is accomplished by simply dividing COLD (1-3) by NHIT .

For a positive T2 , there are two cases , the energy of M before the collisions above ETHRESH and below ETHRESH .

When the original $E_m > ETHRESH$ and there was only one collision , the co-ordinates of M are set to the DEV results , and a jump is made to the next box . If there was more than one collision , E_m is set equal to T2 , and the velocities are scaled so that the components will be in the same proportion as the sum of the individual resultant velocities as computed by the subroutine . This essentially gives M a resultant direction equal to the vector sum of the directions M would have as a result of its collisions with the rest of the KHIT list .

When the original $E_m \leq ETHRESH$, we assume that M has been oscillating about a site , and its site number is obtained from LB (M) . E_m is then set equal to T2 , and the velocities are scaled so that the resultant velocity vector will point toward M's oscillatory center . The scaling factor is $(V^2 / (\Delta X^2 + \Delta Y^2 + \Delta Z^2))^{1/2}$. This is multiplied by ΔX , ΔY , and ΔZ to obtain the correct components . This scaling automatically keeps V^2 in proper proportion to E_m .

BOX 21

TLAST for M is calculated at the start of this box . M's TLAST

could not be calculated before this point since M had not yet participated in all its possible collisions.

This box then insures that all atoms with energies less than ETHRESH have site numbers stored in LB, that they are placed on the LATER list if their energies are less than THERMAL, or that they are left alone if in between the two thresholds.

If an atom has $E > \text{ETHRESH}$, its site number must be removed from LB (M), and the bit signifying an occupied site must be removed from LB (site), unless the atom was once part of an interstitial pair. If it was part of an interstitial, then the partner section of LB must be removed from both LB's.

If an atom should occupy a site and doesn't, then a site must be found. This is accomplished by going part way through INVAC, INVAC is exited by use of the MOVE indicator. If a site is calculated for M, and it is occupied, the information pertinent to an interstitial pair is recorded in LB. If the site is occupied by an interstitial, M is placed on the site anyway, and the fact that a "triple interstitial" was formed is recorded by increasing MISTAKE (5). E_m is inspected at this point, and MISTAKE (3) is increased if E_m is negative. The symbolic language of this box may appear complicated, but comprehension should be facilitated by the flow chart.

BOX 22

All other atoms on the KHIT list are now subjected to the same process M underwent in the previous box, except that here a jump is made

to Statement 600 to enter INVAC. To preserve the values of I, J, and M, and also make M equal J, the values of I, J, and M are stored in MAD, NAVY, and LOCATE, respectively. These two boxes might, at some future stage of development be combined into one box covering the entire KHIT list. However, when this section was developed, the treatment of M and the others on the KHIT list was sufficiently different so that this combination would have been prohibitively difficult. Most of this difficulty has disappeared as the program developed.

BOX 23

All atoms on the KHIT list are now backed up, time-wise and space-wise, to the beginning of the current time step. Each atom must be backed up using its particular T (), since they were not all hit at exactly the same time. A search through the NUM list accomplishes this, giving the correct value on the T list for the computation.

BOX 24

If one of the J's on the KHIT list was a member of an interstitial pair, then NPAIR is three, and a jump is made to Statement 236. The relations between atom M (the incoming atom), atom J (the member of the pair struck by M), and the partner, atom LL (the other member of the interstitial pair), are now considered.

If J has an energy between the two thresholds (vibrating about its site), the information in LB about it must be retained. If the partner, LL, has been hit, and has an energy greater than ETHRESH, the MASK1 portion of both LB's must be erased. If both have an energy \leq ETHRESH,

nothing is done to either LB. If, however, J has an energy greater than ETHRESH and atom LL has not been hit, we must erase from LB (J) the site and partner number, erase from LB (LL) LL's partner number (which is J), and also move atom LL back onto the site. It would be a definite error to leave the partner, LL, on its previous split position, so it seems more realistic to move it back onto the site.

BOX 25

The interactions, scaling, and correction of LB have now been completed for this round of collisions. A jump is now made to Statement 200 in BOX 16. If M has no more collisions this time step, a jump back to this point will be made. If M does have further collisions, they are calculated and carried out.

Upon entering this box, if IN3 is zero, then no collisions were made during the last pass through, and this M has completed the time step. The next atom on the LAST list, the INMINth one, is made atom M. INMAX is the limit of this list. INMIN is increased by one, and a jump is made to Statement 200. When the LAST list has been exhausted, i.e. each one has been through the process until it will have no more collisions this time step, an exit to the next box is made.

Any atoms on the LAST list that have been put on the LATER list to go through INVAC are not sent back through the collision process since they have MASK6 set.

The name of the atom under primary consideration was changed from L to M in BOX 15 to prevent the above process from destroying the value

of L, since L is the index on the main DO loop over the atoms.

BOX 26

In a DO loop over the LAST list, only those atoms not on the LATER list are selected, and then moved to the end of the time step. This fact is then recorded in LB. The atom's energy is then compared with ENERGY, the largest one becomes the new ENERGY, and INERGY is changed if needed.

BOX 27

If $NZ = 1$, the LATER list is empty, and a jump is made around this box. If not, IT1 is set equal to $(NZ - 1)$, as the upper limit of the DO loop to follow. INVAC is then called successively for all of the LATER list, writing on Tape 6 in binary the particle number and time step, both contained in IU, and the X, Y, and Z co-ordinates.

BOX 28

In this DO loop on J, only those atoms on the LAST list that were not on the LATER list (and have consequently been through INVAC) are considered.

All three co-ordinates are compared to the lattice dimensions. If an atom is outside the physical dimensions of the lattice, a value of NFACE is calculated. NFACE and the number of the time step of exit are then recorded in LB (M), the site number and possible interstitial partner are erased from LB (M), and M's number is erased from any interstitial partner's LB. The memory of occupancy is erased from the site if M is not an interstitial member, and the next atom on the LAST

list is considered.

This is the end of the major DO loop on L, the next L is chosen, or an exit is made to the next box if the DO loop on L is completed.

BOX 29

The same procedure is followed here as was followed in BOXES 26 and 28 above, except that atoms:

- 1) That have been through the time step,
- 2) Having an energy less than THERMAL, or,
- 3) That are outside the lattice

are not considered.

This is the end of the major DO loop on N, the time step is completed, and either a new time step is started, or an exit to the next box and the output section is made.

BOX 30

Writes selected lattice and program parameters, and a general lattice dump on Tape 8 in binary for eventual use by the SLAVE program. Various BCD output is then written on Tape 3, and if the DO loop on N (the time steps) was completed, a (-1) is written in binary on Tape 6 and the program ends. If, however, the DO loop on N was not completed, a jump is made back to BOX 11. There, a jump is made back to this box (with the resultant (-1) on Tape 6, etc.) if Jump Switch 3 is not set. In the normal operational mode, the DO loop is not completed, and the program itself terminates computation by a jump from BOX 11 to the start of this box, the output is written, the jumps back to BOX 11 and back are made, and

the program ends .

A jump around the BCD section of the output may be made by setting Jump Switches 1 & 3. To facilitate resetting of the jump switches, Stop Switch 1 may be set. If this is done, the program will stop after writing Tape 8, and again before jumping back to BOX 11.

Tapes 3 & 4, then, are used for BCD output, and Tapes 6, 7, and 8 are used for binary output over the course of a run (including regeneration). Since Tape 4 output is normally switched to the typewriter, only four output tapes are needed in the course of a run. The three binary tapes (6,7,8) will be rewound at the end of the run, and may be used without further action. An END OF FILE mark must be placed on the end of Tape 3 before printing.

SUBROUTINE SITE (M)

BOX 31

This short subroutine calculates the fixed point co-ordinates of the lattice site given as an input parameter. The co-ordinates are found in IB (1-3) after exit from the subroutine.

SUBROUTINE INVAC (MJ)

This subroutine, given the number of an atom, either places the atom on a vacant lattice site near it, or forms an interstitial pair with one of its nearest neighbors.

BOX 32

The initial indicator IN2 is set to zero, and the input atom is changed to number MM. The site number occupied by MM, and the fact

that MM is on the LATER list are now cleared from LB (MM), and the fact that MM has gone through INVAC is set in LB (MM).

Atom MM's co-ordinates are now inspected to see whether or not MM is within one unit of a face of the lattice. If so, the number of this face is stored in IFACE (1-3), and the indicator NIF is increased. The index of IFACE is 1, 2, or 3, depending on whether the face is in the X, Y, or Z direction, respectively.

The co-ordinates of MM are rounded off, and the fixed point co-ordinates of the nearest site (or non-site) are found.

BOX 33

We must now determine which of the two general cases we have, site or non-site, and if IFACE (1-3) is non-zero, which of the 12 special cases we are to consider. If the sum of the three fixed point co-ordinates is even, then they designate a lattice site, and JM is set to 1. If the sum is odd, then a non-site is designated, and JM is set to zero. The sum of the Y and Z co-ordinates is then checked. If odd, JL = 0, and if even, JL = -1. If the indicator MOVE is non-zero, a RETURN to the main program is executed.

The formula for IL (the site number) results in an X co-ordinate one less or one more than an actual site for the non-site case. The sum of JL and JM determine which case. If the sum is -1, then one is added to IL.

At this point, IL is always either:

- 1) The site of the rounded off position of MM, or

2) The site with X co-ordinate one larger than MM's rounded-off position.

The possible special case is now determined. If IFACE (1-3) $\neq 0$, then JB is set equal to the face number with JD = 1. If more than one IFACE is non-zero, MISTAKE (2) is increased, since this means a position along an edge or corner of the lattice.

In either case, if IFACE (1-3) $\neq 0$, then JA is non-zero, and JC is set equal to 1. If IFACE (1-3) is zero, then JC = JM (either 1 or 0). JB is set equal to the first non-zero IFACE or to zero if IFACE (1-3) is zero. JD is then set to 1 if a non-zero IFACE exists, and to zero otherwise.

The case number (1-14) is now established by the formula:

$JW = (JM*6*JD) + 1 + JB + JC$. Cases 1 & 2 are the general cases.

Cases 3-8 are special forms of case 1, with cases 9-14 as special forms of case 2. These special cases simply eliminate some of the nearest neighbors found in the general case from consideration.

The lists MOON and NOON are set to zero, and the next box is entered.

BOX 34

The first section (down to Statement 2451) is a section of computed GO TO statements to insure the correct choice of the nearest neighbor formulas. The second section places the site numbers of the nearest neighbor positions on the MOON list, provided their numbers lie between one and MAXLAT. I is the index used for the MOON list, and is always

one greater than the number of sites on the list.

BOX 35

All of the nearest neighbor numbers found may not have been placed on the MOON list (possible negative numbers, or numbers greater than MAXLAT). JPMAX, therefore, is reset to (I-1). If the indicator MOVE is non-zero, a RETURN to the main program is executed.

The LB for each atom whose site is on the MOON list is now inspected. If the LB shows that the site is not occupied (see APPENDIX I), the site number is placed on the NOON list. JP is the index used for the NOON list.

The MOON list, then, is a list of the sites of the nearest neighbors, and the NOON list is a list of those nearest neighbor sites that are vacant sites, with JK the number of vacancies on the NOON list.

BOX 36

If $JK = 1$, then only one vacancy exists, and atom MM is placed there, the site number, IL, is set in LB (MM), and the fact that the site is now occupied is stored in LB (IL). If IN2 is zero, a RETURN is then executed, otherwise a jump to BOX 39 (Statement 2800) is executed.

If JK is zero, there are no vacancies and a prospective interstitial partner must be found. If IN2 is zero, a jump to BOX 38 is made to accomplish this. If IN2 is non-zero, then MM is the prospective interstitial partner of the original atom MJ, and a jump is made to BOX 39 to form the interstitial.

If $JK > 1$, then more than one vacancy exists. A jump is made to BOX 37, where one of the vacancies is chosen, a return to this box is then made, and the procedure given for $JK = 1$ is followed.

BOX 37

The $(\text{distance})^2$ between atom MM and the vacant sites on the NOON list is computed and stored in the DSTANCE array. The minimum $(\text{distance})^2$ is then found, and the DSTANCE list is inspected to find the number of sites that are at this minimum distance from atom MM. If there is only one, IL is set equal to that site, and a jump is made to Statement 2492 in BOX 36. If there is more than one, MM is placed on its own site, if its own site is one of those on the list. If not, then MM is placed on the first or second site on the NOON list, depending on whether the number of the time step is odd or even, respectively.

The number of the time step is used here as a convenient random number generator, since the decision is made on oddness or evenness, rather than the actual value of the number itself.

BOX 38

This box is entered only from BOX 36, and then on the condition that IN2 is zero and that MM (MJ) has found no vacancies. A prospective interstitial partner must be chosen from the MOON list.

The time of atom MM's (MJ's) closest approach to each of the sites listed on the MOON list is found and stored in the TMIN list. Any sites occupied by interstitial pairs are not considered.

The minimum time of closest approach is then found, TMIN (KMIN), which locates the prospective interstitial site. MAX is derived from ΔX , ΔY , or ΔZ , whichever is greatest ($\Delta X = X$ co-ordinate of MM minus X co-ordinate of the site chosen), and this becomes the prospective axis of the interstitial pair. The atom occupying this site is then found. Since it is possible for this atom to be pushed into any vacancy near it, and MM to fall into the vacancy thus created, this atom's nearest neighbors must be inspected. This is done by setting MM equal to the number of this atom, setting IN2 to 1, and jumping to Statement 2361 in BOX 32. BOX 39

If the new MM (the original atom is still designated by MJ) does find a vacancy, it is placed there in BOX 36, a jump is made to this box, MM's now vacant site is named as the prospective site for MJ, a return to BOX 36 is made, and MJ is placed on its prospective site. A RETURN to the main program is then executed in BOX 36.

If, however, the new MM did not find a vacant site, then a jump is made to this box (Statement 2720), and the interstitial is actually formed. The site of the interstitial is entered in each LB, together with the other atom's number. The fact that the site is occupied is then entered in the LB of the site, and a RETURN is executed.

If the new MM equals MJ, then the atom has formed an interstitial with itself, and the error counter MISTAKE (4) is increased. The interstitial is formed so that MJ is on the same side as it was before formation of the interstitial pair.

SUBROUTINE INTER (MQ, II, S)

This subroutine, given the atom under consideration (MQ), the target atom (II), and the impact parameter (S, in meters) calculates the positions of the atoms at the end of the collision, their velocities, and energies and stores them in the DEV array.

BOX 40

Transforms atom MQ's position co-ordinates, velocity components, and energy and the angle between the radius vector from atom II to atom MQ and MQ's velocity into the target (atom II) frame of reference. Sets CPA = SPHI as the initial value for the CPA iteration.

BOX 41

Computes CPA by an iterative process. The iteration is terminated when two successive values differ by less than 10^{-4} %, or when any value is greater than the preceding value.

BOX 42

Computes the time required for the interaction and the total angle of deviation. The integrals are solved by numerical integration using a Gauss-Legendre four point quadrature.

BOX 43

Computes the composite factors and trigonometric functions that are used more than once in the transformation to the laboratory reference frame.

BOX 44

Computes direction cosines, relative to the laboratory frame of

reference, of a line in the plane of the interaction that is perpendicular to the line between the two atoms at the beginning of the interaction.

BOX 45

Computes the position co-ordinates, velocity components, and energies of both atoms and stores them in the DEV array. See APPENDIX I, DEV for the actual location.

PROGRAM SLAVE

BOX 1

Reads binary input from Tape 8. "SET SLJ SWITCH 2 UP IF NEEDED" is written on Tape 3 (normally transferred to the typewriter). As many comment cards (80 spaces per card) as desired (6 at present) are read from Tape 2 and written on the output tape. Reads input parameters for the run from Tape 2. Writes on the output tape "SELECTIVE JUMP SWITCH NUMBER TWO WAS UP" if Jump Switch 2 is used for the run.

IHISTO (1-4) and IHISTO (105) are defined, the IHISTO array then serves as the format specification for the histograms. The constants I2E15, I2E24, F2E24, and I2E30 are set, and the masks for use with the LB array are defined.

BOX 2

If NTS (called N in PROGRAM MASTER, the number of time steps completed) is zero, then NTS is set equal to MNTS; other constants and indicators are then set. The times in the TSLI array and the time TSL are converted from jiffys to seconds. Various portions of the LB array are then cleared, depending on the settings of the jump switches.

BOX 3

In this box all atoms are placed in one of the following classifications:

- 1) Atoms occupying their original sites ,
- 2) Atoms occupying sites other than their original sites ,
- 3) Atoms that are parts of interstitial pairs ,
- 4) Atoms whose energy is greater than ETHRESH , and
- 5) Atoms outside the lattice .

Program MASTER has also calculated the face of exit for those atoms that have left the lattice .

The number of atoms and the total energy of those atoms is calculated for each classification , as is the number of vacant lattice sites .

BOX 4

The total number of atoms and their total energy is calculated. This serves as an additional total energy check at the end of the computational run. These numbers and various other data (see APPENDIX III) are written on the output tape. The number of atoms and their total energy is written on the output tape for each classification listed in BOX 3.

BOX 5

The number of atoms occupying their original sites is written on the output tape. An array of these atoms is then written , in order , on the output tape. Atoms not on their original sites are represented by zeros in this array.

BOX 6

The total number of vacant lattice sites and the numbers of these sites are written on the output tape.

BOX 7

The total number of replacements is written on the output tape. The number of the atom, the number of its final site, its penetration, and its radial penetration are written on the output tape for each of the replacement atoms. Histograms are then compiled and written on the output tape for the penetration and the radial penetration distributions of the replacement atoms.

BOX 8

The total number of interstitial pairs is written on the output tape. The number of each atom in a pair, its partner, the site they occupy, the penetration of each atom in the pair, and the radial penetration of each atom in the pair is written on the output tape. This is written twice for each interstitial pair since there are two atoms in the pair. Histograms are compiled and written on the output tape for the penetration and the radial penetration distributions of all interstitial pair members.

If Jump Switch 2 was set for the run, the interstitials are determined by inspecting the LB array given by program MASTER. If, however, Jump Switch 2 was not set, the program disregards the LB array and calculates the interstitial pairs in the lattice.

BOX 9

The total number of atoms with energy greater than ETHRESH

(knock-ons) is written on the output tape. The number of each atom, its co-ordinates, velocity components, energy, its LB (in octal), its penetration, and its radial penetration are written on the output tape for each knock-on atom. Histograms are then compiled and written on the output tape for the penetration, radial penetration, and energy distributions of the knock-on atoms.

BOX 10

The total number of atoms that exited through a lattice face is written on the output tape. The number of the atom, its co-ordinates, its velocity components, energy, LB (in octal), its penetration, radial penetration, and time step of exit are written on the output tape for each atom exiting through a face.

The entire box is then repeated for each of the six faces of the lattice.

BOX 11

If Jump Switch 1 is set, a jump is made to the end of the program, otherwise a general lattice dump is written on the output tape. The dump consists of the atom number, co-ordinates, velocity components, energy, and the LB contents (in octal) for each atom.

SUBROUTINE ROUND (L)

BOX 12

This subroutine computes the site closest to atom L. The atom's co-ordinates are rounded off, and the fixed point co-ordinates of the atom are stored in the IB array if the co-ordinates represent a site.

If the fixed point co-ordinates do not represent a site, the six nearest neighbor sites are found. The site that is closest space-wise to the atom is chosen as the site for atom L. Once a site is chosen, a RETURN to the main program is executed.

SUBROUTINE INITIAL (L)

BOX 13

If atom L is one of the original lattice atoms, this subroutine computes its initial fixed point co-ordinates and stores them in the IB array. If atom L was shot into the lattice, the point of entry is stored in the IB array. A RETURN to the main program is then executed.

SUBROUTINE ECOUNT (L)

BOX 14

The energy of atom L is inspected. This energy will fall between two of the values on the KET list, say the sixth and the seventh values on the list. Atom L's energy is then greater than the sixth (Ith) value on the list. The histogram counter IC (I + 50) is then increased by one. A RETURN to the main program is then executed.

SUBROUTINE DEPTH (L)

BOX 15

The penetration (DEPTH) is computed as the final X co-ordinate of atom L minus the initial X co-ordinate. A value of I is determined so that DEPTH lies between A (I - 7.5) and A (I - 6.5). Histogram counter IC (I) is then increased by one.

The radial penetration (PERDIST) is then calculated from L's initial and final positions. A value of I is determined so that PERDIST lies between A (I - 1) and A (I). Histogram counter IC (I + 30) is then increased by one. A RETURN to the main program is then executed.

SUBROUTINE HISTO (NGROUPS)

BOX 16

The largest number and the total of NUMBERS (1 -NGROUPS) are determined. The total is written on the output tape. The percentage of the total is written on the output tape for each entry on the NUMBERS list, followed by a number of X's corresponding to the percentage this entry is of the largest number in the table, i.e. the largest number will write out 100 X's, and a number half that large will write out 50 X's. A RETURN to the main program is then executed.

PROGRAM RON

This program writes on the output tape the successive positions of every atom in the lattice (or that was shot into the lattice), if the successive position of an atom is significantly different from the previous position. The number of the time step is also written when an atom's co-ordinates are written. After writing all the successive positions of an atom, the program commences writing the positions of the next atom that has moved significantly until all atoms have been considered.

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