NAVAL POSTGRADUATE SCHOOL
Monterey, California

THESIS

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Richard David Williams III

Thesis Advisor: D.E. Harrison, Jr.

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Richard David Williams III
Lieutenant Commander, United States Navy
B.S., United States Naval Academy, 1964

Submitted in partial fulfillment of the
requirements for the degree of

MASTER OF SCIENCE IN PHYSICS

from the

NAVAL POSTGRADUATE SCHOOL
December 1972

ABSTRACT

Computer simulation techniques were used to determine equilibrium positions and binding energies of inert gas atoms implanted in a tungsten crystal and to investigate the potential wells around these equilibrium positions in both perfect lattices and relaxed lattices. Stable positions were found for inert gas interstitials near lattice atoms in the third and fourth layers of the crystal. Interstitial positions near atoms in the first and second layers of the crystal appeared to be unstable if they exist at all. As a result of potential well studies, it was concluded that the mechanism associated with equilibrium position formation was a combination of local liquefaction of the lattice structure and interaction of the interstitial with lattice atoms. Equilibrium positions were found to be ill-defined regions in the general ⟨110⟩ direction. The binding energy determined for an interstitial site near a lattice atom in the third layer of the crystal was in excellent agreement with experimental results.

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I. INTRODUCTION

In 1968 Kornelsen and Sinha [1] of the National Research Council of Canada published results of radiation-damage experiments performed on tungsten. In these experiments a tungsten surface was bombarded with ions of neon, argon, krypton, and xenon respectively. Then, while the tungsten was heated, gas desorption rates were measured as the gas evolved from the crystal. The resultant desorption spectrum was interpreted to yield a binding energy spectrum for the trapped particles. In 1970 Professor Don E. Harrison, Jr., of the Naval Postgraduate School undertook the modeling of these experiments utilizing computer simulation techniques in order to provide a means for interpretation of their results. Two successive thesis research efforts [2,3] have been specifically directed toward the investigation of inert gas implantation in a tungsten crystal. It was anticipated that a corollary to the successful computer simulation of this problem might possibly be an improved understanding of the interstitial atom stabilization mechanism in tungsten, with more general application to other materials.

The investigations reported in this paper are a continuation of work begun by Vine [2] and Tankovich [3] under Harrison's supervision. The simulation procedures followed were a combination of static and dynamic approaches to the problem. The static portion of the problem entailed

interstitial implantation of an inert gas atom in a tungsten crystal and the subsequent relaxation of the crystal until the equilibrium position of the interstitial could be ascertained. In the dynamic portion of the problem decreasing amounts of energy were imparted to the interstitial in its equilibrium position until the minimum energy, and direction, which still allowed the interstitial to escape from the crystal was determined (i.e., the binding energy of the particle). The binding energies thus determined provided a basis for comparison with the results of Kornelsen and Sinha.

II. THE NATURE OF THE PROBLEM

A. THE LATTICE DYNAMICS PROBLEM IN THE COMPUTER

For a little over a decade high speed digital computers have exhibited their usefulness as tools for investigation of physical systems. Specifically, the inherent periodicity and order of crystal lattices have made the study of lattice dynamics particularly adaptable to investigation by computer simulation. It is a relatively simple matter to "construct" a crystal of the desired body-centered cubic or face-centered cubic structure in the computer. Various types of point defects can also be "created" in the crystal with relative ease. A vacancy is obtained by simply removing an atom from the crystal, while interstitials can be created by implanting an additional atom in the crystal. Two types of interstitials have been used in investigations of lattice dynamics, atoms identical to the crystal lattice atoms ("self-interstitials") and atoms different from the crystal lattice atoms (interstitials).

Although a crystal lattice containing a point defect can be easily represented in a computer, modeling of the dynamics, which allows alterations of the crystal structure resulting from the presence of the point defect, is more involved. The dynamic portion of the problem of computer modeling of lattices can be characterized by four key decisions which must be made.

First, it is necessary to find some mathematical relationship to govern the interaction among the atoms of the crystal. This interaction is a complex many body problem which is nearly always approximated in computer simulations as a sum of appropriate two body interactions. With this approximation it is then possible to represent these two body interactions by some type of potential function, which, in turn, can be used to determine forces on individual atoms.

Secondly, since the number of calculations required is directly related to the number of atoms in the crystal, a judicious choice of crystal size must be made. Large crystals would give more accurate results, but would also require more computational time.

A third key problem which must be solved results from the inability of a digital computer to perform a direct integration. Since the lattice dynamics problem is most often directed at a determination of lattice atom positions after some type of interaction, an integration of the equations of motion is required. A choice of the numerical integration technique to be used must therefore be made.

Last, and probably most important, since an iterative process is used to integrate the equations of motion, the length of the time interval of the iteration must be chosen so that the force variations within this time interval are small and, consequently, stability of the system is insured. At first glance, this suggests that only very small timesteps should be taken, but this would require excessive computer

time. Consequently, some variational method of timestep determination would be optimum.

B. HISTORICAL DEVELOPMENT OF COMPUTER SIMULATION OF LATTICE DYNAMICS

The four basic problems of computer simulation of lattice dynamics have been solved in various ways in previous investigations.

In 1960 Gibson, Goland, Milgram, and Vineyard [4] (referred to hereafter as Gibson, et.al) of the Brookhaven National Laboratory published the first complete statement of computer simulation procedure as a tool for investigation of radiation damage of crystal materials. Due to the complexity of the radiation damage problem and the inadequacy of analytical methods as a means of analysis of the damage processes, Gibson, et.al. turned to a numerical integration of the problem utilizing high speed computers. Their pioneering work gives insight into such pertinent subjects as crystal size, choice of potential functions, computational methods for solving the equations of motion, and timestep determination.

Specifically, their research utilized copper as the crystal material since its relatively simple face-centered cubic structure and its widespread use in actual experimentation made it particularly appropriate for initial investigation. A Born-Mayer repulsive potential was used to describe atom-atom interaction, and a constant cohesive force was applied to each atom on the crystal surface to balance the

Born-Mayer repulsion. A central difference iterative procedure was used to integrate the equations of motion. The procedure used for timestep determination is of particular significance since the principles involved are still the governing criteria for choice of timestep duration. The fundamental observation was made that the greatest stress on the crystal system was a result of the strongest atom-atom interaction in the system. This interaction was therefore chosen as the basis for timestep determination. Simply, the timestep duration was chosen to be inversly proportional to the velocity created by the strongest atom-atom interaction.

In addition to verifying the applicability of computer simulation techniques to radiation damage studies and providing specific information on collision chains and focusing phenomena in crystallites, the work of Gibson, et.al.[4] determined that the only stable configuration for self-interstitials in a face-centered cubic crystal was the ⟨100⟩ split configuration. The split configuration implies that the interstitial causes a lattice atom to split away from its normal lattice position, and then both atoms, the interstitial and the lattice atom, share (or split) the normal lattice site when equilibrium is reached.

Johnson and Brown [5] confirmed the split configuration as the only stable interstitial position in their studies of copper utilizing a Born-Mayer repulsive force between nearest neighbors and an elastic continuum containing the remainder of the atoms of the crystal. Erginsoy, Vineyard,

and Englert [6] (referred to hereafter as Erginsoy, et.al.) extended these calculations to the body-centered cubic case by performing investigations using α iron. Computational techniques paralleled those of the Brookhaven group except for the choice of a potential function. After experimentation with a Born-Mayer potential and a Morse potential with parameters derived by Girifalco and Weizer [7], Erginsoy, et.al. [6] settled on a combination potential which utilized an exponentially screened Coulomb potential for close approaches, a Born-Mayer potential for first nearest neighbor, and a Morse or modified Morse potential for higher order neighbors. This research verified the split configuration as the only stable configuration for body-centered cubic structures, but the orientation of the split was found to be in a (110) plane, (vice a (100) plane as in the face-centered cubic case). R.A. Johnson [8] confirmed the split interstitial orientation in similar work with α iron, vanadium and tungsten.

In their work on collisions between a copper atom and a copper lattice, Gay and Harrison [9] introduced the average force procedure for integrating the equations of motion. A complete description of this procedure has been reported by Gay, Effron, and Harrison [10]. In two more recent efforts Johnson and Wilson [11,12] determined new potential functions for use in face-centered cubic and body-centered cubic defect calculations and published results of defect calculations of helium in various metals.

Parallel to the computer simulation efforts described above, Kornelsen [13,14] and Kornelsen and Sinha [1,15] have published the results of extensive experimentation involving the interaction of inert gas ions with tungsten. Under Harrison's supervision, Vine [2] initiated attempts to devise a computer model of Kornelsen's experiments on neon implantation in tungsten. He attempted to develop a relationship between equilibrium positions of tungsten interstitials in a tungsten crystal determined, first, by using a Born-Mayer repulsive potential to describe tungsten interstitial interaction with a tungsten lattice then, by using the same tungsten-tungsten composite potential which was assumed between atomsof the tungsten crystal. This relationship would then have been applied to neon equilibrium positions derived from a repulsive potential to provide a comparison with Kornelsen's data. These efforts met with little success.

Follow-on work by Tankovich [3] utilized the static/dynamic approach described in more detail in Section III-B. The potential function used in these investigations was a composite Born-Mayer and Morse potential joined by the best cubic fit in the area of intersection which had previously been developed by Harrison and Moore [16]. Static program runs confirmed the ⟨110⟩ split interstitial for helium, neon, argon, krypton, and xenon point defects in a tungsten crystal for possible interstitial sites in planes three through six of the ten plane crystal used. Preliminary

dynamic testing of an argon equilibrium position in plane four of the crystal was begun with limited success.

Of particular significance in Tankovich's work [3] was the introduction of a timestep decrementing process into the static program. In previous investigations the timestep duration was chosen at the outset of the problem and remained constant through all computations. At this author's suggestion, a timestep decrementing process was devised which allowed a more rapid approach to the equilibrium positions with a concomitant saving of computer time required for computation. (See Section III-A-3 for a discussion of the timestep.)

III. THE SIMULATION PROCEDURE

A. THE MODEL

1. The Crystal

Two factors are of primary importance in determining the size of the crystal to be used in computer simulation investigations. First, the crystal must be large enough to provide realistic results, and, second, the crystal must be as small as possible in order to minimize computer time required for calculation of atom-atom interactions.

After experimenting with crystals of various sizes, Tankovich [3] determined that a crystal with ten planes of atoms in each coordinate direction, which is equivalent to five unit cells, (10 x 10 x 10) was suitable for static investigations with tungsten. The same crystal was consequently used in the investigations reported in this paper. The lattice unit, or distance between adjacent (100) planes of atoms, for a body-centered cubic tungsten crystal is 1.58Å. All distances in the computer simulation were measured in lattice units. The lattice constant for the tungsten crystal is 3.16Å (or two lattice units), and the nearest neighbor distance is $\sqrt{3}$ lattice units.

The same numbering sequence for atoms of the crystal that was employed by Tankovich [3] was used in these investigation. (See Figure 1.) Atom number one was always assigned to the interstitial atom. A rectangular coordinate system was placed on the upper, left hand, front face of the crystal.

The positive "x" direction was chosen to the right from the origin, the positive "y" direction was down, and the positive "z" direction was to the rear. Atoms were numbered consecutively, beginning with atom number 2 at the origin and continuing until all atoms of the Y = 0 plane had been numbered. This same numbering sequence was then followed for each Y plane of the crystal until all 250 atoms of the crystal had been numbered. Figure 1 shows the numbering of the atoms in the Y = 0 and Y = 1 planes. The numbering of atoms in the remainder of the planes follows the same pattern.

For the dynamic program it was felt that a smaller crystal could be used and still yield meaningful results. The rationale for this determination was based on the go-no go (i.e., escape or no escape) character of the dynamic program. The dynamic program essentially provides an answer to this question - Will an interstitial atom escape from the crystal if it is given a specific energy and directed in a specific direction? If the energy dissipation mechanism provided by collisions with, and close approaches to, the lattice atoms along the path traveled is great enough, the interstitial will remain in the crystal. If these energy dissipation mechanisms are not large enough to overcome the kinetic energy of the interstitial, the interstitial will escape. Since the atoms of the crystal along this line of motion must provide the mechanism to dissipate the interstitial's kinetic energy, for escape to be prevented, only atoms in the horizontal planes above the interstitial and atoms in vertical planes within a few lattice units of the

interstitial will affect the possible escape. The remainder of the atoms of the crystal would not have time to react with the interstitial or affect its movement. As a minimum, the smaller crystal could be used to eliminate excessively high or low energies from consideration at a considerable savings of computer time and, instead, give a limited range of energies to be checked by dynamic runs using the entire crystal.

To implement this procedure SUBROUTINE PLUCK was developed. (See Appendix A for a complete discussion of SUBROUTINE PLUCK.) Basically, SUBROUTINE PLUCK uses the results of the static program, but causes a crystal to be printed out that only contains the interstitial and all lattice atoms from two planes below the interstitial to the surface plane of the crystal and all atoms in vertical planes which are within two (or three) lattice units of the vertical plane containing the lattice site shared by the split interstitial. (See Figure 2.) The savings in computer time resultingfrom the use of this smaller crystal is demonstrated by the following comparison. A thirty timestep dynamic run with the entire 10 x 10 x 10 crystal (250 atoms) used approximately three and one half minutes of computer time. A thirty timestep dynamic run using a 7 x 5 x 7 crystal (60 atoms) used slightly less than one minute of computer time - a 71% savings in computer time!

Most of the dynamic runs made during the course of these investigations utilized the 7 x 5 x 7 "PLUCK" crystal. Final confirmation of minimum energies was determined using the entire crystal.

2. The Potential Function

As mentioned previously, the many-body interaction which characterizes actual lattice dynamics is approximated in computers by many two-body interactions. These two-body interactions are represented in the computer by some type of central, pairwise potential function. Various types and combinations of potential functions have been considered for use in computer simulation investigations of lattice dynamics.

The choice of the potential function must be made with due consideration to the range of applicability of the potential function, the correlation of potential function parameters with observable properties of the material being investigated, and the amount of computer time required for calculations using that potential function. The potential function used in these investigations was the composite Born-Mayer potential and Girifalco and Weizer Morse potential used by Tankovich [3,16]. This composite potential is constructed as follows:

a. Region 1-($r < 1.5Å$)

The atom-atom interaction at close approach is represented by a Born Mayer repulsive potential of the form,

$$\Phi_{ij} = \exp(A+B\ r_{ij}) \tag{1}$$

where Φ_{ij} is the interaction energy between particles i and j and r_{ij} is the distance between particles i and j.

b. Region 2-($1.5Å < r < 2.0Å$)

This portion of the potential function is obtained by computing the best cubic equation between the value

of the Born Mayer potential at 1.5Å and the value of the Morse Potential at 2.0Å.

c. Region 3-(2.0Å $<$ r $<$ 5.38Å)

For equilibrium and greater separations, a Morse potential of the form,

$$\Phi_{ij} = D[\exp\{-2\alpha(r_{ij}-r_o)\} - 2\exp\{-\alpha(r_{ij}-r_o)\}] \tag{2}$$

where Φ_{ij} is the interaction energy between particles i and j, D is the dissociation energy of the particles i and j, r_{ij} is the distance between particles i and j, and r_o is the equilibrium separation, is used. The Morse potential was computed so that the tail of the function was truncated to zero at 5.38Å. This effectively meant that atoms out to the fourth nearest neighbor were included in calculations of interaction energies. Girifalco and Weizer [7] had previously determined Morse potential parameters for tungsten and other elements which included interactions out to the 150th nearest neighbor. Use of the complete function, however, would have required an excessive amount of computer time for calculation. Additionally, contributions to the interaction energy of all atoms beyond the fourth nearest neighbor is essentially insignificant for our calculations. Many computer simulations of lattice dynamics of body-centered cubic materials have utilized potential functions which only included first and second nearest neighbors with satisfactory results [6,11]. To check the adequacy of this potential function in describing this crystal system, the

largest binding energy observed in the crystal model (-8.283 eV) may be compared with the experimentally determined heat of sublimation for tungsten (-8.8 eV) reported by Harrison and Magnuson [17]. This agreement within 5.9 percent was considered satisfactory for these simulations.

3. The Timestep

a. General Discussion of the Timestep

Most of the early simulations of lattice dynamics used a central difference method as the numerical procedure of integrating the equations of motion of the atoms in the crystal. See Gibson, et.al [4] or Gay, Effron and Harrison[10] for an explanation of the central difference method of numerical integration. The investigations reported in this paper, however, used the average force method which is completely described by Gay, Effron, and Harrison [10]. Inherent to both numerical methods of integration is the replacement of time derivatives in the equations of motion with a finite time difference, i.e., the timestep interval. As mentioned previously, the strongest interatomic interaction places the greatest demand on the system; consequently, the timestep duration is usually determined through consideration of the strongest interatomic interaction of the system. These investigations followed the procedure of Gay, Effron, and Harrison [10] and determined the timestep duration by a consideration of the maximum displacement that the most energetic atom of the crystal was allowed to move. This parameter, referred to hereafter and in all computer programs as DTI, is determined as follows:

(1) The equation of motion of i^{th} atom of the crystal during timestep interval ΔT can be written in the form

$$x_i(t+\Delta T) = x_i(t) + [v_i(t) + \langle F_i \rangle \Delta T/2m]\,\Delta T \qquad (3)$$

or in the equivalent form

$$\Delta x_i = (v_i + \langle F_i \rangle \Delta T/2m)\,\Delta T. \qquad (4)$$

(2) Rearranging terms of equation (4) yields

$$\Delta T = \Delta x_i/(v_i + \langle F_i \rangle \Delta T/2m) \qquad (5)$$

where ΔT is the timestep interval, Δx_i is the displacement of the i^{th} atom during the timestep, v_i is the velocity of the i^{th} atom, and $\langle F_i \rangle$ is the average force on the i^{th} atom.

From equation (5) it can be seen that the timestep interval is a function of both the kinetic energy and the force. Rather than solving this quadratic equation for the timestep interval, the average force method considers separately the cases when energies dominate forces ($v_i >> \langle F_i \rangle \Delta T/2m$) and when forces dominate energies ($\langle F_i \rangle \Delta T/2m >> v_i$). Solutions for each of these cases yields a different value for the (next) timestep interval.

In energy dominant cases,

$$\Delta T = \Delta x_i/v_i \qquad (6)$$

or, expressed in the form of energies,

$$\Delta T = \Delta x_i (m/2T_m)^{-\frac{1}{2}} \qquad (6a)$$

and, in force dominant cases,

$$\Delta T = (2m\ \Delta x_i/\langle F_i \rangle)^{\frac{1}{2}}, \qquad (7)$$

where T_m of equation (6A) represents the kinetic energy of the atom of the crystal with the greatest kinetic energy, and $\langle F_i \rangle$ of equation (7) represents the average force on the atom with the maximum force, the Δx_i of each equation becomes DTI.

In these investigations, DTI was set at the beginning of the program. Ideally, the proper choice of timestep duration for the first timestep and the proper choice of DTI would lead to a smooth movement of the interstitial to its equilibrium position in a manner similar to the movement of a critically damped oscillator.

It was anticipated that energies would dominate forces in early timesteps which would lead to timestep determination from the energy equation, equation (6A). At some point in the crystal relaxation procedure, energies should have been dissipated to the point where further timestep determination would become force dependent (equation (7)).

b. The Average Force Method and Timestep Determination

In the average force method of integration of the equations of motion, velocities (i.e., energies) of, and forces among, all atoms of the crystal are computed with the atoms in their initial positions. Based on these forces and energies and the initial timestep duration, new positions for all atoms of the crystal are computed. The forces at the new positions are then averaged with the forces at the original positions to determine the average force, and hence the final positions of all atoms at the end of the first timestep.

In the meantime, the maximum force exerted on an atom of the crystal in its original position and the maximum force exerted on an atom of the crystal in its final (averaged) position are used with the DTI and equation (7) to calculate two possible alternatives for the next timestep interval. Likewise, the energies of the most energetic atoms in both original and final positions are used with DTI and equation (6A) to calculate two other possible alternatives for the next timestep interval. These four alternatives are then compared, and the smallest is chosen as the next timestep interval.

c. Procedures Used to Determine DTI

Vine[2] utilized a constant DTI in all of his computations. Since the movement of an interstitial to an equilibrium position cannot, in general, be characterized by a small range of energies and forces and since DTI should be closely correlated <u>with</u> energies and forces at least in appropriate regions, the use of a constant DTI in all calculations made the initial choice of DTI extremely critical. Success could only be attained by resorting to small DTI's and concomitant excessive program run times (≥ 100 timesteps).

Tankovich [3] obtained more satisfactory results by successively decrementing DTI for each timestep. This procedure allowed long timesteps in early portions of a run when the interstitial was far from its equilibrium position. As equilibrium was approached, the decrementing process had progressed to the point such that significantly smaller and smaller timesteps were taken allowing a smooth arrival at the

equilibrium position. Additionally, this was accomplished at a considerable savings of computer time (~ 30 timesteps).

Although this decrementing process for DTI provided considerable improvement, on occasion, the final few timesteps used such a small DTI that practically no atom movement was discernible. During these investigations this situation was alleviated by incorporating a minimum DTI into the decrementing process. This insured that atom movement was still discernible near equilibrium and assisted in guarding against possible false assumption of equilibrium because of the relatively small movement observed under the continuous decrementing process.

In an attempt to more fully understand the mechanisms of the static solution, the computer program was adjusted so that the maximum force, the atom upon which this force was exerted, and the four "new" possible timesteps for each timestep interval were printed out after each run. It was observed that the timestep calculations based upon "new" and "old" energies were overwhelmingly the basis for timestep determination. To insure that the force dependence of the timestep was not being unduly disregarded, the program was adjusted so that DTI was determined solely as a function of the minimum of the two forces. These "force calculations" of equilibrium positions agreed with "energy calculations" within 0.03 lattice unit.

B. THE PROGRAMS

Although the basic computational procedures contained in the computer programs for the static and dynamic portions of the problem were essentially the same, an understanding of the subtle differences between the programs and an appreciation for several computational tools and procedures used in the programs have to be gained prior to further discussion of the actual investigation and results.

1. The Static Program

In the static program, a tungsten crystal of appropriate size was created in the computer. An interstitial atom was then implanted at a chosen site within the crystal. Potential energies and mutual forces of all atoms were computed. The crystal was then allowed to relax in appropriately chosen timesteps. At the end of each timestep an energy dissipation mechanism was introduced in the form of a predetermined damping factor which was used to decrease all velocity components of the atoms of the crystal. The next timestep interval was then computed, and the process was repeated until an indicated number of timesteps had been completed. If an equilibrium position had been reached, positions and energies of all atoms in the crystal, including the interstitial, and other pertinent data could be punched out on cards for later use in the dynamic program.

a. Equilibrium Positions of Interstitials

In interpreting the results of the static simulations it was necessary to arrive at some criterion to use as a determining factor for the interstitial's final

equilibrium position. It was expected that the crystal would relax around the split interstitial site forming a "pocket" within the crystal which would interrupt the periodicity of the lattice. Stability in this configuration was determined to have been reached when the atoms of the deformed crystal, including the interstitial, had been allowed to relax (i.e., adjust to the presence of the interstitial) to the point where their kinetic energies were all below thermal. (< 0.025 eV)

If more than one possible equilibrium position met this criterion, it was felt that different positions within the "potential well" of the equilibrium site were probably being observed. The position in which the interstitial atom had the smallest amount of potential energy was then chosen as the equilibrium position for the lattice site under investigation.

b. Handling of Oscillations Near Equilibrium

While performing the "force calculations", some runs began with the interstitial moving toward an apparent equilibrium until an oscillation, or "rattle", developed about the suspected equilibrium position in the "z" direction. It was first confirmed that this "rattle" was solely in the "z" direction (i.e., no significant "x" or "y" displacement) by extending the computation from 30 to 200 timesteps. It was shown that in a ⟨100⟩ direction in a body-centered cubic a narrow potential energy minimum was observed at (100) planes. The region of the ⟨110⟩ line between the octahedral void and the reference lattice site was contained within

this potential energy minimum. With this information as justification, it was determined that the velocity of the interstitial in the "z" direction could be completely damped at the end of each timestep to hasten the determination of the true equilibrium position. This technique was useful in restricting computer run time whenever an obvious "rattle" in the "z" direction developed.

2. The Dynamic Program

The initial step of the dynamic program was the re-creation in the computer of the tungsten crystal, including the interstitial, after relaxation of the crystal had taken place and the interstitial had come to an equilibrium position. This was accomplished by utilizing the output of the static program as the input to the dynamic program.

Before continuing with the problem, it was necessary to realize that the minimum energy required for the interstitial to escape from the crystal would be a function of the path of escape. To account for this "direction dependence", impact points were chosen in the surface plane of the crystal perpendicular to the direction of escape. The negative "y" direction was always used as the direction of escape. Energy was then imparted to the interstitial which was, in turn, "aimed" at a specific impact point. The interstitial was then allowed to travel through the crystal using a timestep procedure based on a constant DTI. (The timestep procedure in the dynamic program is simpler than in the static program since energies are dominant throughout.) Each impact point (i.e., direction of escape) was subsequently

tested in the same manner using the same initial energy. If the interstitial escaped from the crystal in any direction tested, it was assumed that the initial energy applied to the interstitial was greater than the binding energy for that particular ion in that particular equilibrium position. In this case, the initial energy was decreased and another survey of the impact points was taken. When the minimum initial energy which still allowed the interstitial to escape was determined, the binding energy for that particular ion in that particular equilibrium position was known.

3. Equilibrium Sites Viewed As Potential Wells

One means of modeling equilibrium positions of interstitials in a crystal lattice is to consider each possible equilibrium position as a three dimensional potential well. A foreign atom migrating through the lattice which reaches the confines of one of these potential wells with sufficiently small energy would fall into the potential well and remain there. In conjunction with this research, the character of these potential wells was also investigated.

Two different approaches were taken to investigate the potential well aspect of the problem. First, the static program was used to investigate behavior of interstitials implanted at various positions around a previously determined equilibrium position in a perfect lattice to determine which of these positions sought equilibrium. The second method offset the interstitial from its equilibrium position in the relaxed crystal and then allowed the crystal to undergo

further relaxation to determine whether the offset interstitial would seek the original equilibrium position.

4. Determination Of Possible Interstitial Sites

In a body-centered cubic material there are twelve possible locations for a ⟨110⟩ split interstitial. In an infinite crystal these sites are equivalent; that is, no one site can be distinguished from another. When a finite crystal is considered, the presence of a crystal surface allows identification of three distinct interstitial sites. An "A" site is located in a (110) plane which contains the lattice site about which the split occurs and is closer to the crystal surface than the shared lattice site. A "C" site is also in a (110) plane containing the shared lattice site, but is located below the shared lattice site. A "B" site is located in the same (100) plane parallel to the surface that contains the shared lattice site.

a. Implantation Procedure

In the static program the interstitial was initially implanted in an offset position in the direction of the expected equilibrium position. This procedure allowed a smooth movement toward the suspected equilibrium position in a minimum number of timesteps. For the heavier interstitial atoms (xenon and tungsten) the lattice atom was also offset in its direction of suspected movement as a result of the presence of the large interstitial.

IV. PRESENTATION OF DATA

A. STATIC SIMULATION

1. Initial Simulations

After the minimum DTI procedure had been incorporated into the DTI decrementing process, investigations of tungsten interstitials in a tungsten crystal were made. In particular, a comparison between tungsten movement under the influence of an attractive potential and tungsten movement under the influence of a repulsive potential was sought. Equilibrium positions determined separately with these two potentials gave agreement within 0.02 lattice unit.

Investigations were then extended to verify equilibrium positions near lattice sites 89 and 64 which had previously been obtained by Tankovich [3]. Positions for argon, neon, krypton, and xenon were examined for each site, and results agreed with Tankovich's data within 0.02 lattice unit, see Table I. As the mass of the interstitial atom decreased, its equilibrium position moved from the shared lattice site location previously reported [7,8] toward the center of the octahedral void.

2. Site 39

Investigations were then directed toward determining equilibrium positions of a split interstitial near lattice site 39, which is one layer below the surface of the crystal. Calculations were made separately for argon, neon, krypton, and xenon interstitials. At the end of thirty timesteps,

TABLE I

Interstitial and Lattice Atom Displacements from Reference Site

Interstitial	Interstitial Site	Interstitial Displacement		Lattice Atom Displacement	
		Δx	Δy	Δx	Δy
Neon	89C	-0.86	+0.87	+0.06	-0.06
Argon	89C	-0.80	+0.80	+0.19	-0.19
Krypton	89C	-0.77	+0.77	+0.24	-0.24
Xenon	89C	-0.48	+0.48	+0.41	-0.42
Tungsten	89C	-0.38	+0.39	+0.35	-0.35

all atoms of the crystal in each case had kinetic energies below thermal, which indicated that an equilibrium had been reached. An observation was made, however, that tended to abrogate this determination. The lighter interstitials, neon and argon, exhibited a definite affinity for the surface of the crystal. In all three possible sites (A,B, and C), argon and neon interstitials were found to seek positions significantly (~ 0.1 lattice unit) closer to the surface than the expected ⟨110⟩ split. Final positions for argon and neon interstitials in site 39A were located less than three tenths of a lattice unit below the surface of the crystal. Similar behavior, but to a lesser degree, was also observed with the heavier interstitials, krypton and xenon. Additionally, although the kinetic energy criteria indicated that an equilibrium had been reached, the small velocities that were available at the end of each timestep were in such a direction as to allow escape from the crystal if these velocities could be maintained. In fact, although velocities were halved at the end of each timestep, a comparison of velocities over the last five timesteps of the computer run showed that the negative "y" (direction of escape) velocity component of the interstitial at the end of timestep thirty was actually only twenty percent lower than the same velocity component at the end of timestep twenty five. In other words, even with fifty percent damping applied during <u>each</u> timestep, velocities actually decreased by only twenty percent over <u>5</u> timesteps. It was also observed that during these last five timesteps the

maximum movement allowed by the most active atom of the crystal (the DTI) had reached its minimum value, 0.0005 lattice unit. These observations suggested that the small movement allowed during these timesteps combined with the damping factor might be "forcing" the interstitial to exhibit equilibrium criteria. It was concluded that equilibrium positions near site 39 were unstable, if they exist at all.

3. Site 14C

Until these investigations little thought was given to the possibility of an equilibrium position in site 14C. With no precise knowledge available concerning the actual quantitative value of the damping experienced by a foreign interstitial implanted in a crystal lattice and with the possibility of equilibrium sites near lattice site 39, some credence had to be given to the possibility of equilibrium positions near surface atoms of the crystal. It was, therefore, decided to investigate the possibility of an equilibrium position in site 14C. It was postulated that in the case of light atoms (neon, for example) the interstitial position for the 14C site should be deeper in the crystal than the 39A site, as a result of the greater repulsion of the lattice atom with which the site was shared. Simulations showed that the 14C interstitial site was located at a distance of 0.43 lattice unit below the surface of the crystal while the 39A interstitial site was located at a distance of 0.26 lattice unit below the crystal surface. When the displacement of this interstitial site was compared

with the 64C interstitial site (0.84 lattice unit below the next higher lattice plane), the effect of the surface of the crystal on interstitials in close proximity to the surface was clearly exhibited. Velocity characteristics similar to those of site 39A were also observed indicating that the amount of damping applied and the DTI could be forcing the interstitial to exhibit equilibrium properties in this site. In general, it can be said that interstitial equilibrium sites in the first two layers of the crystal are ill defined in position if they exist at all.

4. Force Calculations

As mentioned previously, in the course of these investigations it was determined that energies nearly always dominated forces for the timestep ranges used in the calculations, and, consequently, the timestep was nearly always chosen as a function of the energy of the most energetic atom. To ascertain whether the use of timesteps determined by maximum forces would yield better or significantly different results, the static program was modified so that the timesteps were determined strictly as a function of the maximum force. This was accomplished by first printing out the maximum force observed during each timestep. By surveying these maximum forces, several values of force were chosen to be used as test forces. As the program was subsequently run, the maximum force in each timestep was compared with these test forces, and a DTI for that timestep was assigned based on the results of that comparison. This assigned value of DTI was then used to compute the next

timestep interval. These calculations of equilibrium positions based on forces agreed with previous energy calculations of equilibrium positions within 0.03 lattice unit.

It should be realized here that the terminology "force calculations" and "energy calculations" do not imply any significant difference <u>in method</u> for determining equilibrium positions. They are merely two different procedures for determining the maximum displacement which will be allowed by the most energetic atom of the crystal during the next timestep. The importance of this parameter (DTI) is in the effect it has in insuring the smooth movement of the interstitial to its equilibrium position.

5. Investigation of Potential Wells

Viewing interstitial equilibrium positions as potential wells of varying depths is a convenient means of modeling the entrapment of foreign atoms by lattice structures. In order to minimize the effects of the crystal surface on investigations, interstitial site 89C, which had exhibited good stability and almost perfect $\langle 110 \rangle$ splitting in previous testing, was chosen for investigation of the characteristics of interstitial potential wells.

a. Potential Well Studies in a Perfect Lattice

The first approach to the study of the interstitial potential well utilized essentially the same method that had been originally employed to locate equilibrium positions. It was postulated that any interstitial atom that was implanted in a perfect lattice at or near the coordinates of

the equilibrium position which had been previously determined for interstitial site 89C would seek the same equilibrium site. Interstitial atoms could be implanted further and further from the previously determined equilibrium position until they no longer returned to it. In this manner a map of the size of the potential well around site 89C could be obtained.

The results obtained in investigations of xenon in site 89C are presented in Figure 3. In this figure each coordinate intersection represents an implantation site which was tested. The arrows drawn from these implantation sites indicate the direction of movement of the interstitial from that specific implantation site. The tip of the arrow represents the interstitial position after thirty timesteps.

In considering the data obtained in these investigations, two significant observations were made. First, an interstitial implanted at the previously determined equilibrium position (coordinates (4.52, 3.48) in Figure 3) moved from this position to another position which also met the criteria for equilibrium. Secondly, all other implantation sites also moved to positions which met equilibrium criteria. An analysis of the program print out data provided information of secondary importance. All implanted atoms exhibited an initial movement in the general ⟨110⟩ direction even though final positions were not necessarily in that direction. Similar investigations were conducted using argon and neon interstitials with similar results.

In light of this unexpected behavior in the perfect lattice the stability of a foreign atom, inserted into the crystal as a replacement for the lattice atom in site 89, was examined. Investigations were made using neon, argon, krypton, and xenon as the replacement atoms. The data from these runs are tabulated below.

TABLE II

Results of Replacement Runs in Site 89

Replacement Atom	Y Displacement (L.U.) After 30 Timesteps	Final Kinetic Energy (eV)	Final Potential Energy (eV)
Neon	-0.049	0.0000	1.0444
Argon	-0.036	0.0008	3.5118
Krypton	-0.029	0.0001	3.5120
Xenon	-0.020	0.0000	1.3297

The y displacement values are sufficiently small that site 89 must be presumed to be a stable replacement site. This conclusion is further confirmed by observing that the potential energies are also significantly lower than those obtained for the same atoms when acting as interstitials, see Table III.

TABLE III

Interstitial Potential Energies for Site 89C

Interstitial Atom	Final Potential Energy (eV)
Neon	4.7
Argon	16.3
Krypton	15.5
Xenon	9.1

To further check the stability of this site, a kryptron replacement atom was then initially offset from the site 89 coordinates, 0.7 lattice unit in the "x" and "y" directions, and the program was run again. The krypton atom moved precisely along the ⟨110⟩ line back toward site 89. At the end of thiry timesteps, the krypton atom was located 0.4 lattice unit in the "x" and "y" directions, "x" and "y" velocity components were still in the direction of site 89, and potential energy had decreased from 54 eV in the initial offset position to 8.7 eV at the end of thirty timesteps.

(1) Interpretation of Results

Interpretation of the results reported in the previous section led to a re-examination of the concept of the equilibrium positions of interstitials and raised a question concerning the validity of solely using relaxed crystals for determinations of equilibria.

The equilibrium positions obtained by using a perfect crystal were a function of the implantation site. This dependency of the final equilibrium position on the implantation site suggested that the movement of the interstitial to an equilibrium site can not be explained in terms of the lattice structure "forcing" the interstitial to its lowest energy configuration. Rather, these results suggested that the actual mechanism is a process of local "liquefaction" of the lattice as it adjusts to the presence of the interstitial <u>combined with</u> interstitial movement caused by interaction with the lattice atoms. This, in turn,

suggested that a more accurate means of localizing equilibrium positions might be to utilize a crystal which had already been allowed to "relax", or adjust to the presence of the interstitial. (See next section.)

The movement of atoms from nine different implantation sites in an area two tenths of a lattice unit per side to nine different positions which exhibit equilibrium criteria indicated that equilibrium positions are not precise positions coordinate - wise within the time range of these computations.

b. Potential Well Studies in a Relaxed Lattice

The conclusions reached as a result of studies of potential wells in a perfect crystal prompted similar studies in a crystal which had been allowed to adjust to the presence of the interstitial. An argon interstitial and interstitial site 89C were chosen for investigation. The relaxed lattice was obtained by using the results of the static simulation of argon in site 89C which had first indicated that an equilibrium position had been reached. These results were read into the computer as initial positions for the lattice atoms and the interstitial. The interstitial was then offset from its position and a new static simulation was performed. An array of sites was chosen for investigation in this manner. The results of these simulations with various interstitial offsets are shown in Figure 4. The representation in Figure 4 is analogous to the representation in Figure 3. The start point for each run is numbered (1-9 and A,B).

The interstitial movement depicted in Figure 4 was encouraging in many respects. An argon interstitial placed successively at each initial site (numbered 1-9 in Figure 4) appeared to head for roughly the same region of the crystal. The potential energy of the interstitial at the conclusion of each run ranged in value from 8.8 to 9.8 eV. A comparison of these energies with the energy of the interstitial in the initial equilibrium position found in the perfect lattice (~16 eV) indicated that this equilibrium region is much more stable than the position determined previously. While not precisely defined in position, this equilibrium region was located in roughly the ⟨110⟩ direction from the shared lattice site.

Since this equilibrium region appeared to be located nearer to the shared lattice site (site 89) than offset start points 1-9, two additional computer runs (labeled A and B in Figure 4) were made with start points bordering this equilibrium region. These runs indicated that, even in a relaxed crystal, the equilibrium reached was still somewhat a function of the initial position of the interstitial. In both of these runs, equilibrium was reached by movement in the ⟨110⟩ direction, and the potential energy of the interstitial after thirty timesteps (~ 10 eV) was lower than the potential energy originally determined in the perfect lattice.

(1) Interpretation of Results

The results obtained in the relaxed lattice seemed to reinforce the conclusions drawn during the study

of potential wells in the perfect lattice. Basically, the relaxed crystal studies gave a picture of equilibrium positions much more in tune with what might reasonably be expected in nature. It seems clear that the equilibrium site of an interstitial is an ill-defined region in the general ⟨110⟩ direction from the shared lattice site. Determination of this equilibrium region cannot be made based solely on the kinetic energy of the interstitial; potential energies must also be considered.

This equilibrium region could have been postulated from a consideration of the rms displacement of a tungsten atom in a tungsten lattice. Houska [18] has measured this rms displacement to be 0.049 lattice unit at 300°K. The ordinary thermal activity of the lattice atoms, then, can be expected to cause the equilibrium positions of interstitials to fluctuate over some region. This equilibrium region might best be described as roughly a cylinder whose axis is in the ⟨110⟩ direction and whose height and radius are some function of the relationship between interstitial mass, lattice atom mass, and the interatomic potential function. The equilibrium positions determined in these investigations appeared to be centered in the ⟨110⟩ direction at the intersection of the (110) and (100) planes through the lattice atom and covered a section of the ⟨110⟩ line on the order of 0.2 of a lattice unit long. This seems to be a reasonable range of equilibrium positions for the relatively light argon interstitial in a tungsten crystal.

The results of these investigations have indicated the usefulness of conducting implantation studies in relaxed crystals. The movement of interstitials to equilibrium in the relaxed crystal was much less dependent upon initial positions, and all sites investigated showed a preference for positions in the ⟨110⟩ direction. Such was not the case in perfect lattice studies.

B. DYNAMIC SIMULATIONS

Concurrent with the investigations into the potential wells of the equilibrium sites, dynamic simulations were conducted using the argon interstitial in site 64A. Since Tankovich [3] had investigated an argon interstitial in site 89C and had determined that the binding energy of this site was in the range 2-4 eV, 4 eV was chosen as the initial energy for the dynamic tests. It was determined that the binding energy of the argon interstitial in site 64A was between 0.02 and 0.04 eV. At 0.04 eV escape of the interstitial was noted for several of the twelve impact points tested. At 0.02 eV the interstitial first moved slightly toward the surface of the crystal, then changed directions and moved to a position deep inside the crystal while gaining considerable energy. This phenomena had been seen and interpreted previously as the expected behavior of a stable site in which the interstitial has been required to move too large a distance in one timestep. Since the timestep is constant (0.1 lattice unit) in the dynamic simulation, an interstitial that is oscillating in a stable configuration

can be required to move out of its stable position. When this movement is directed into the crystal, it can be assumed that the original position was stable.

This binding energy falls in the range of the first desorption peak measured by Kornelsen and Sinha (see Figure 5 in Ref. 1). This result indicated that interstitial sites formed with lattice atoms in the third crystal plane (corresponding to the y = 2 plane of these calculations), such that the interstitial site was in the ⟨110⟩ direction <u>above</u> the lattice atom, are the sites nearest the surface of the crystal stable enough to entrap measurable amounts of argon. This excellent concurrence with experiment further substantiated the conclusion drawn earlier in these investigations about the doubtful character of positions near sites 39 and 14 which had exhibited equilibrium criteria.

V. CONCLUSIONS AND RECOMMENDATIONS

During the course of these investigations the possibility that the DTI decrementing procedure and the procedure for incorporating damping into the problem might be forcing interstitials to exhibit equilibrium properties arose. At first, the DTI was thought to possibly be restricting atom movement to such an extent during the last few timesteps of a calculation (i.e., when DTI had reached its minimum value -0.0005 lattice unit) that atom movement and, consequently, kinetic energy could no longer be used as equilibrium criteria. This became more significant when the small DTI and the damping factor were considered together. The damping factor seemed particularly appropriate for scrutiny near the surface of the crystal and when DTI was small, since the probability of collisions and close approaches and the subsequent damping of atom motion could be expected to decrease in both instances. The excellent agreement with experiment of the results of the dynamic and static simulations suggests, however, that the DTI and damping procedures employed might be adequate for these simulations except when atom movement is particularly close to the surface of the crystal. It is recommended that future investigations explore the use of a damping factor which varies with decreasing DTI and movement toward the surface of the crystal.

These investigations have shown the value of using a relaxed crystal in the computer simulation of lattice dynamics. The relaxed crystal simulation indicated that:

(1) The equilibrium position initially sought by an interstitial is a function of implantation position.

(2) The mechanism associated with the establishment of an equilibrium position seems to be a combination of interatomic interaction and local liquefaction of the crystal structure in the vicinity of the interstitial.

(3) The character of equilibrium potential wells is more readily observable in a relaxed crystal.

(4) The actual equilibrium position of an interstitial seems to be some region in the general ⟨110⟩ direction from the reference (shared) lattice site.

Again, however, for determining binding energies, the original procedure for determining equilibrium positions may yield adequate results. Such was the case for the dynamic simulations reported here. It is recommended that replacement interstitials and other split interstitial sites undergo dynamic simulation in an attempt to correlate other desorption peaks as determined by Kornelsen and Sinha [1] with interstitial sites.

APPENDIX A

SUBROUTINE PLUCK

Subroutine Pluck was developed to allow the use of a crystal smaller than the original model in dynamic testing. This subroutine was developed so that the only pieces of information required as input to the subroutine were the number of crystal planes desired in the "x" and "z" directions and the number of the lattice site desired at the center of the PLUCK crystal. Once the size of the PLUCK crystal is decided upon, the subroutine stores the original numbers of the atoms in the PLUCK crystal in an array. This allows reference to any atom by its original number throughout computation. The atoms of the PLUCK crystal were numbered consecutively, and the number of atoms in the PLUCK crystal was assigned a variable name. In this manner, a minimum of adjustment was required in the dynamic program when the PLUCK crystal was used.

SUBROUTINE PLUCK is included in this appendix in its most general form. Parameters are listed below for two different sizes of PLUCK crystals. Sizes refer to the number of "x" and "z" planes in the PLUCK crystal. "Y" planes from the surface of the crystal through the two planes below the plane of the lattice site under investigation are always included.

PLUCK PARAMETERS FOR DIFFERENT SIZED CRYSTALS

(crystal sizes refer to number of planes of atoms in x and z directions)

Parameter	7 x 7 Crystal	5 x 5 Crystal
IXNEW	7	5
IZNEW	7	5
NM1	5	3
NI1	8	14
NX1	16	4
NII31	10	16
NII41	5	9
NIINC1	1	3
IIINC1	4	2
NMINC1	4	2
NXINC1	9	9
NMINC2	-1	1
NX2	9	9
NM2	4	4
NI2	8	8
NII32	4	10
NII42	11	15
NIINC3	2	2
IIINC2	3	3
NMINC3	3	3
NXINC2	16	4
NMINC4	1	-1

```
          ************************************
                    'SUBROUTINE PLUCK'
          ************************************

      COMMON/COM1/RX(500),RY(500),RZ(500),LCUT(500),
     1LL,LD,ITYPE,NVAC
      COMMON/COM4/IX,IY,IZ,SCX,SCY,SCZ,IDEEP,D1X,D1Y,D1Z,
     1IVACX,IVACY,IVACZ
      COMMON/COM10/IXNEW,IYNEW,IZNEW,II
      COMMON/COM11/RXNEWI(250),RYNEWI(250),RZNEWI(250),
     1KEEP(250),NNUM(250)
1500  IXNEW=IXNEW
      IYNEW=IVACY+3
      IYNEW=IYNEW
      NM=NM1
      NI=NI1
      II=2
      MM=0
      NX=NX1
      NII3=NII31
      NII4=NII41
      IF(IYNEW.EQ.3) GO TO 1514
      IF(IYNEW.EQ.5) GO TO 1514
1505  DO 1509 I=II,NM
      NNUM(I)=NI
1509  NI=NI+1
      NI=NI+NIINC1
      II=II+IIINC1
      NM=NM+NMINC1
      IF (II.LE.NX) GO TO 1505
      NX=NX+NXINC1
      NI=NI+NII4
      MM=MM+1
      IF(IYNEW.EQ.MM) GO TO 1600
      NM=NM+NMINC2
      GO TO 1515
1514  NX=NX2
      NM=NM2
      NI=NI2
      NII3=NII32
      NII4=NII42
1515  DO 1520 I=II,NM
      NNUM(I)=NI
1520  NI=NI+1
      NI=NI+NIINC3
      II=II+IIINC2
      NM=NM+NMINC3
      IF(II.LE.NX) GO TO 1515
      NX=NX+NXINC2
      NI=NI+NII3
      MM=MM+1
      IF(IYNEW.EQ.MM) GO TO 1600
      NM=NM+NMINC4
      GO TO 1505
1600  II=II-1
      RXNEWI(1)=RX(1)
      RYNEWI(1)=RY(1)
      RZNEWI(1)=RZ(1)
      KEEP(1)=1
      NNUM(1)=1
1700  DO 1750 I=2,II
      RXNEWI(I)=RX(NNUM(I))
      RYNEWI(I)=RY(NNUM(I))
      RZNEWI(I)=RZ(NNUM(I))
      KEEP(I)=NNUM(I)
1750  CONTINUE
      RETURN
      END
```

APPENDIX B

COMPUTER PROGRAM GLOSSARY

ALPHA: Input Morse potential parameter.

BSAVE: Target Mass/ (target mass + bullet mass); distributes potential energy between target and bullet.

BIND: Negative of the total potential energy (TPOT) at time zero.

BMAS: Mass of bullet in AMU.

BULLET: Alpha-numeric array for point defect material.

CFO, CF1, CF2: Force parameters of cubic fit between Morse and Born-Mayer functions.

CGB1, CGB2: Morse potential parameters.

CGD1, CGD2: Morse potential parameters.

CGF1, CGF2: Morse force parameters.

CPO, CP1, CP2, CP3: Potential parameters of cubic fit between Morse and Born-Mayer functions.

CVD: CVR X 10^{-10}: Converts lattice units to meters.

CVE: 1.6 X 10^{-19}: Converts electron volts to Joules.

CVED: CVE/CVD: A ratio used to avoid repeated division.

CVM: 1.672 X 10^{-27}: Converts atomic mass units to kilograms.

CVR: LU in angstroms; converts lattice units to angstrom units.

DIX, DIY, DIZ: Displacement coordinates for location of interstitial from reference atom, NVAC.

DCON: Input Morse potential parameter.

DDTIF: The minimum value that DTI is allowed to assume.

DDTII: The initial decrement of DTI.

DFF: ROE-DIST. The distance closer than ROE that an atom is to the primary.

DIST: Distance between any two atoms.

DLPE: TLPE-TLPE0: The change in total local potential energy since time zero.

DRX, DRY, DRZ: x,y,z components of DIST.

DT: Length of a timestep in seconds.

DTE, DTE1: The two possible alternatives of the timestep computed from maximum energies.

DTF, DTF1: The two possible alternatives of the timestep computed from maximum forces.

DTI: Number of lattice units most energetic atom may move in one timestep.

DT1 (I), DT2 (I), DT3 (I), DT4 (I): Vector arrays which save the possible choices of timestep determined in the "energy" method.

DTSTEP (I): Vector array which saves the timestep interval chosen for each timestep.

DTOD: DT/CVD -- A ratio used to avoid repeated division.

DTOM:DT/PTMAS -- A ratio used to avoid repeated division.

DX(I), DY(I), DZ(I): Change in position of ith atom from initial position at time zero.

EMAX: The maximum energy encountered in any cycle.

EV: Primary energy in electron volts.

EVR: Primary energy in kiloelectron volts.

EXA, EXB: Input Born-Mayer potential function parameters for the target.

F2: Square of the force on a specific atom.

FA: The component force increment on an atom.

FDTI: DTI X CVD: A parameter used to determine DT by maximum energy method.

FM: A small number used in checking potential energy zero point.

FM2: FM squared.

FMAX: Maximum total force on the most stressed atom in the crystal.

FOD: FORCE/DIST: A ratio used to avoid repeated division.

FORCE: Numerical value of the force function with a variable parameter.

FORMAX (I): Vector array which saves the maximum force in each timestep.

FX(I), FY(I), FZ(I): x,y,z, components of total force on an atom.

FAX: Born-Mayer force function parameter.

HBMAS: ½ BMAS: A ratio used to avoid repeated division.

HDTOD: ½ DTOD: A ratio used to avoid repeated division.

HDTOM: ½ DTOM: A ratio used to avoid repeated division.

HDTOMB: ½ DTOMB: A ratio used to avoid repeated division.

HTMAS: ½ TMAS: A ratio used to avoid repeated division.

I1: Variable in cubic fit subroutine.

I3: Variable in cubic fit subroutine.

IDEEP: First fixed layer.

IFMXAM (I): Vector array which saves the atom number which experiences the maximum force.

IH1: Alpha numeric array for program title.

IH2: Alpha numeric array for Morse function parameters.

IHB: Alpha numeric array for bullet element.

IHS: Alpha numeric array for type and orientation of crystal.

IHT: Alpha numeric array for target element.

II: Number of atoms in a crystal using subroutine PLUCK.

ILAY: Number of free (mobile) layers.

IN: Odd-even integer used to determine atom site establishment.

IP: Subscript value of atom. Void in subroutines STEP and ENERGY.

IQ: Parameter that determines whether or not a self defect is to be given a repulsive potential or a composite attractive - repulsive potential.

ISHUT: A parameter used to shut down the program.

IT: Unscaled fixed point x coordinate used in lattice generation.

ITT: Odd-even integer used to determine atom site establishment.

ITYPE: Parameter used to determine the type of point defect: vacancy, interstitial, or replacement.

IX, IY, IZ: Number of x,y,z planes of cyrstal.

IXNEW, IYNEW, IZNEW: Number of x,y, and z planes in the PLUCK crystal.

J2: Variable in the cubic fit subroutine.

JJ: Parameter in the BCC(111) lattice generation subroutine.

JT: Unscaled y coordinate used in crystal generation.

JTS: Variable used to establish atom sites.

JTT: Variable used to establish atom sites.

KEEP (I): Vector array which saves the original atom numbers of the PLUCK crystal.

KF: Final K in LOCAT (K) assigned to an atom.

KT: Unscaled z coordinate used to establish atom site.

LCUT (I): Used to identify an *ith* atom which is not included in calculations.

LD: The highest numbered atom in the mobile layers.

LL: The highest numbered atom in the entire crystal.

LOCAT (K): Dimensioned variable that remembers the numbers of the atoms within a radius ROEL of the primary at time zero.

LS: Variable associated with each of the nine lattice generator subroutines.

MCRO: One number higher than the order of the fit between the Born-Mayer and Morse potentials, always 4 in this simulation.

ND: Data output increment, in numbers of timesteps.

NEW: Parameter used to determine whether or not atom numbers have been stored in LOCAT (K).

NNUM (I): Vector array used in Subroutine PLUCK to re-number atoms.

NPAGE: Page numbering variable.

NRUN: Parameter used to determine whether or not to read additional data cards.

NS: Initial print statement timestep number.

NT: Timestep number.

NTT: Timestep number limit before shutdown.

NVAC: An atom number used to establish point defects or used as a reference point for interstitial placement.

PAC: Parameter for bullet force function correction.

PBMAS: Primary mass in kilograms.

PEXA, PEXB: Input Born-Mayer potential function parameters for the bullet-target interaction.

PFPTC: Primary force function evaluated at ROE.

PFXA: Primary force function parameter.

PKE (I): Kinetic energy of the *ith* atom.

PLANE: Alpha-numeric array for lattice orientation.

POT: Potential energy between two atoms.

PPE (I): Potential energy of the *ith* atom.

PPEINT (I): Vector array that saves the difference in potential energy before and after implantation.

PPENCK: Potential energy check value which determines potential energy decreases which will be printed.

PPENEG (I): Vector array which saves potential energy decreases.

PPEPCK: Potential energy check value which determines which potential energy increases will be printed.

PPEPOS (I): Vector array which saves potential energy increases.

PPESAV (I): Vector array which saves the initial potential energy of lattice atoms before implantation.

PPKEEP (I): Vector array which saves potential energy differences between perfect crystal and relaxed crystal.

PPTC: Primary potential function evaluated at ROE.

PTE (I): Total energy of the *ith* atom (potential + kinetic).

PTMAS: Target mass in kilograms.

RE: Input Morse potential parameter.

RO: Spacing constant in BCC(110) lattice generation subroutine.

ROE: Nearest neighbor distance.

ROE 2: ROE squared.

ROEA: Maximum cut-off for Born-Mayer potential.

ROEB: Minimum cut-off for Morse potential.

ROEC: Maximum cut-off for Morse potential.

ROEC2: ROEC squared.

ROEL: Radius inside of which local potential energy is found.

ROEL2: ROEL squared.

ROEM: ROE-DTI, Region in which modification of repulsive force must be made.

RX(I), RY(I), RZ(I): x,y,z, coordinates of an *ith* atom at any time.

RXI(I), RYK(I), RXI(I): x,y,z, coordinates of an *ith* atom's initial position.

RXK(I), RYK(I), RZK(I): x,y,z coordinates of temporary position of an *ith* atom during force cycle.

RXNEWI, RYNEWI, RZNEWI: Vector arrays which contain the x,y,z, coordinates of the atoms of the PLUCK crystal.

RXSAVE, RYSAVE, RZSAVE: x,y,z, coordinates of the impact point in the dynamic program.

SAVE: ½ POT.

SCX, SCY, SCZ: x,y,z, coordinate scale factors.

SSCZ: A z scale factor used for the FCC(111) lattice generator subroutine.

START: An optional timing variable, not used in this simulation.

SUM: Variable in cubic fit subroutine.

TARGET: Alpha-numeric array for target material.

TSAVE: Bullet mass/(target mass+bullet mass); distributes potential energy between target and bullet.

TE: Total energy of all crystal atoms (kinetic + potential).

TEMP: Temperature of lattice in degrees Kelvin not used in this simulation.

TFAC: A time factor ratio used to determine DT by maximum force method.

TFACB: TFAC for the bullet.

THERM: Thermal energy of atom not used in this simulation.

TIME: Elapsed problem time in seconds.

TLPE: Total local potential energy of atoms within a radius ROEL.

TLPE0: TLPE at time zero.

TMAS: Target atom mass in AMU.

TPKE: Total kinetic energy of all crystal atoms.

TPOT: Total potential energy of all crystal atoms.

VSS: Storage variable for velocity components.

VS(l), VY(l), VZ(l): x,y,z components of ith atoms velocity.

X, Y, Z: Unscaled coordinates used in crystal generation.

XNVAC, YNVAC, ZNVAC: The initial displacement (in LU) of atom NVAC.

YLAX(I): Relaxation in -y direction of ith layer in L.U.

ZP: Floating point form of JTT.

APPENDIX C

ERROR IN THE LITERATURE

It was discovered during the course of these investigations that Equation (20) of Ref. 10 (corresponding to equation 6A of the report) was incorrect.

Equation (19) of Ref. 10 is,

$$\Delta T \doteq \Delta x_i / v_i$$

where ΔT is the timestep interval, Δx_i is the displacement of the i^{th} particle, and v_i is the velocity of the i^{th} particle.

To express the timestep in terms of the energy of the particle with the maximum energy, Δx_i is defined as the displacement of the particle with the greatest energy and is replaced by the symbol D. T_m is this particle's energy, which is the largest kinetic energy at end of each timestep. If T_m is expressed as

$$T_m = \tfrac{1}{2} m v_m^2,$$

substitution into equation (19) yields,

$$\Delta T = D/(2\ T_m/m)^{\frac{1}{2}},$$

or

$$\Delta T = D(m/2\ T_m)^{-\frac{1}{2}}\ ,$$

vice

$$\Delta T = D(2m/T_m)^{-\frac{1}{2}}. \quad \text{(Equation (20) Ref. 10)}$$

It should be noted that this error has no affect on the calculations reported here. D (DTI in these calculations) is a parameter which has been specifically chosen in order

to provide a timestep interval over which there are no significant force changes. The factor of 2 which is introduced in this correction would merely have required a subsequent alteration of the DTI's chosen so that the timestep interval would remain essentially the same.

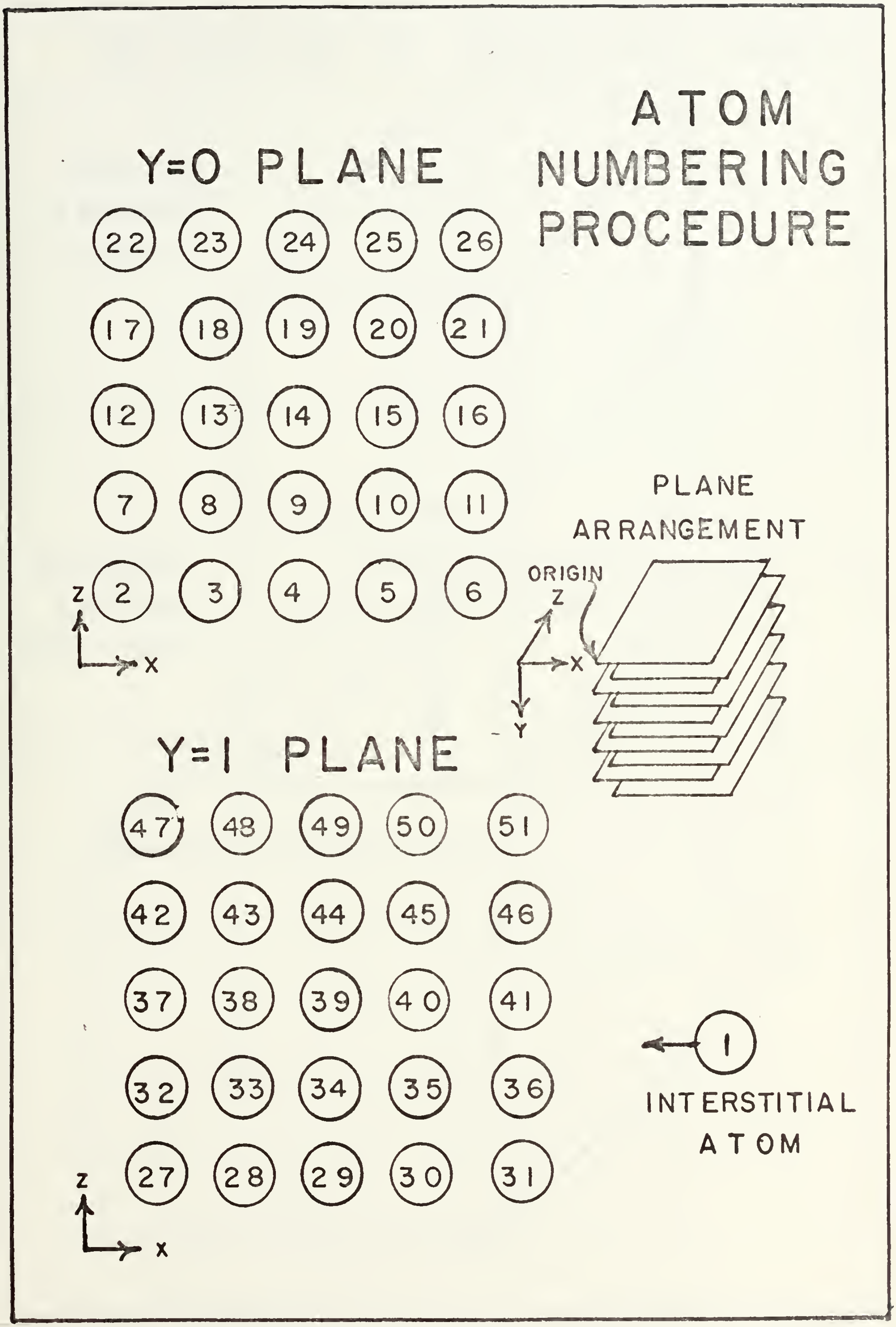

Figure 1. Atom Numbering Procedure.

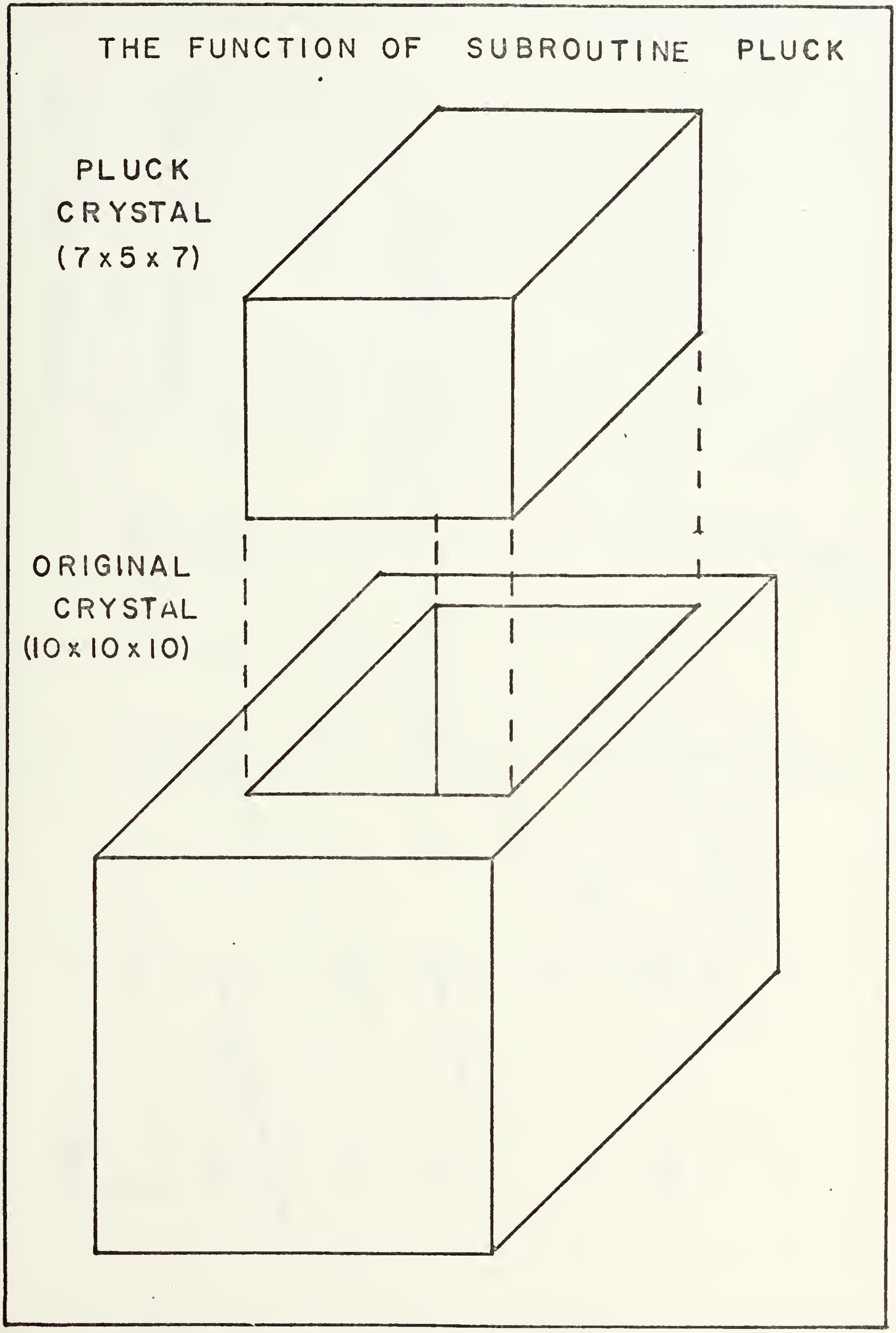

Figure 2. The Function of Subroutine Pluck.

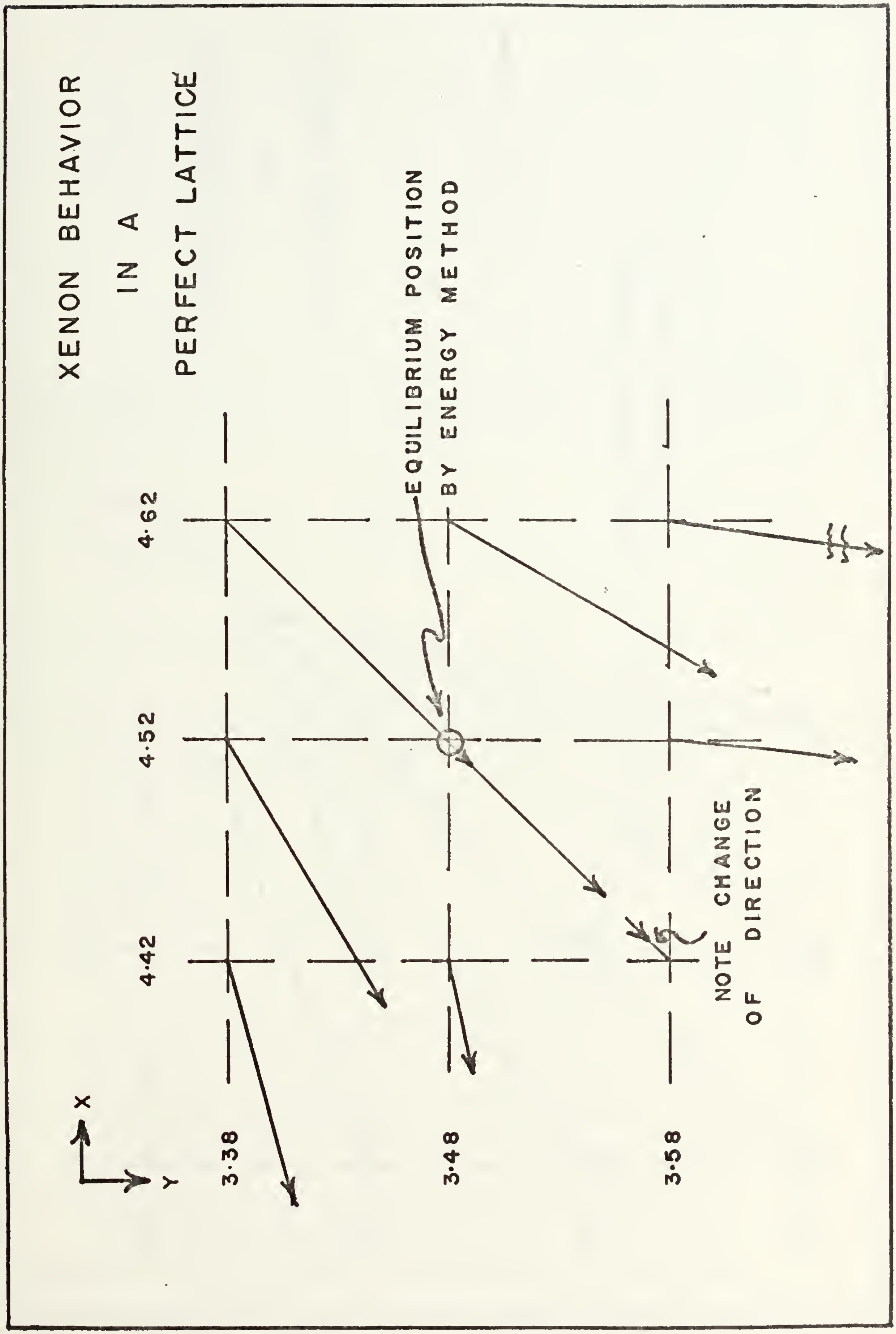

Figure 3. Xenon Behavior in a Perfect Lattice.

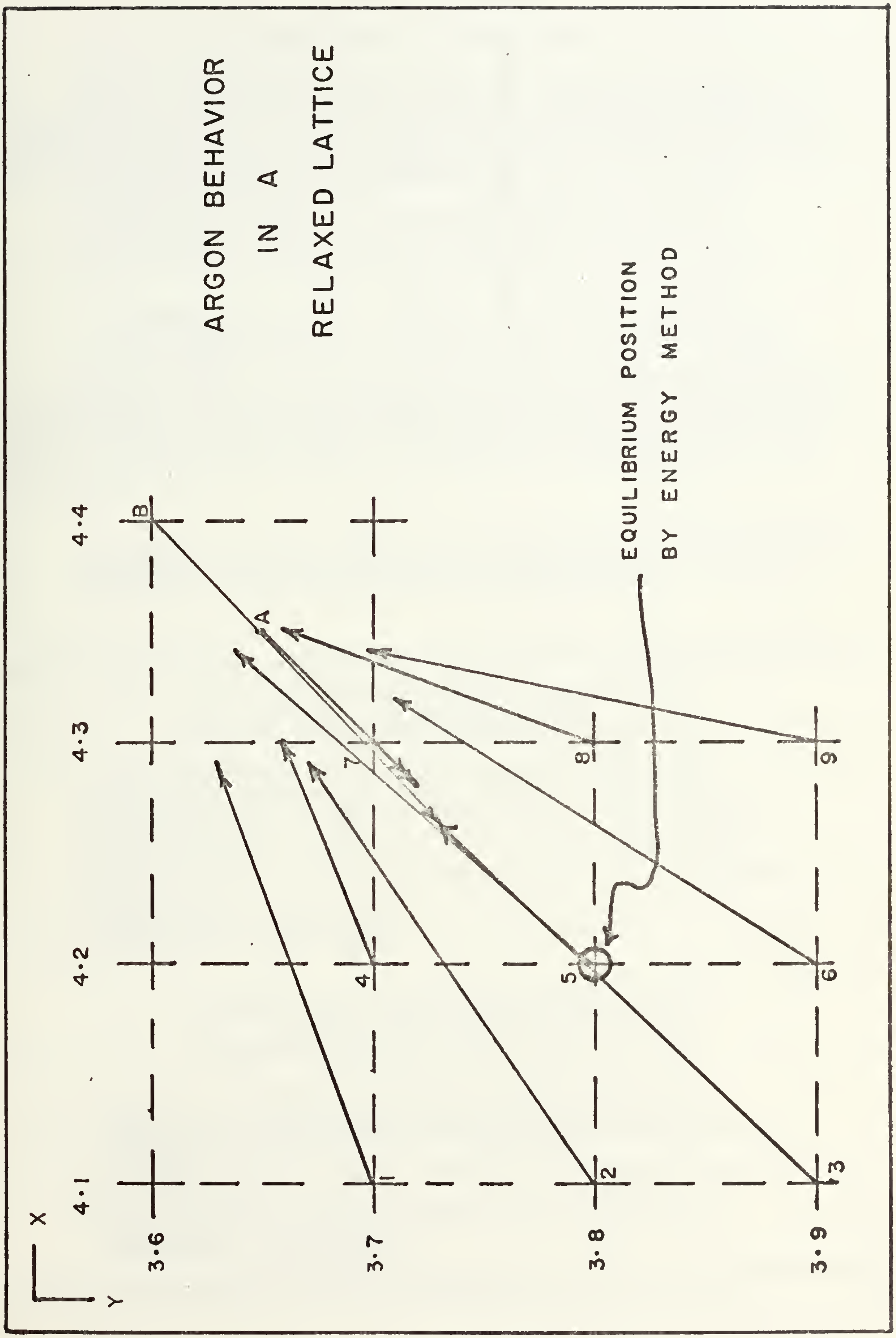

Figure 4. Argon Behavior in a Relaxed Lattice.

COMPUTER PROGRAM

FOR STATIC SIMULATIONS

STATIC SIMULATIONS WERE USED TO INVESTIGATE THE EQUILIBRIUM POSITIONS OF INTERSTITIAL ATOMS IMPLANTED IN A TUNGSTEN CRYSTAL. FOUR DIFFERENT CONFIGURATIONS OF THE STATIC PROGRAM WERE USED AS THE INVESTIGATIONS PROGRESSED. THESE CONFIGURATIONS WERE USED TO

(1) DETERMINE EQUILIBRIUM POSITIONS BY 'ENERGY' CALCULATIONS,
(2) DETERMINE EQUILIBRIUM POSITIONS BY 'FORCE' CALCULATIONS,
(3) PRINT OUT THE SMALLAR CRYSTAL DETERMINED BY

SUBROUTINE PLUCK FOR USE IN INITIAL DYNAMIC TESTING, AND
(4) INVESTIGATE THE POTENTIAL WELLS IN THE RELAXED CRYSTAL.

THE 'ENERGY' CONFIGURATION OF THE STATIC PROGRAM IS PRESENTED BELOW WITH DIFFERENCES FROM THIS PROGRAM REQUIRED BY OTHER CONFIGURATIONS INCLUDED AND DISCUSSED AT APPROPRIATE POINTS. ADDITIONALLY, BRIEF COMMENTS ARE INCLUDED AT VARIOUS POINTS TO CALL ATTENTION TO SIGNIFICANT PROCESSES OF THE PROGRAM.

```
C
C     DIMENSION VECTOR ARRAYS USED EXCLUSIVELY IN THE MAIN
C     PROGRAM. THE DIMENSIONING SCHEME FOR EACH CONFIG-
C     URATION IS GIVEN BELOW IN ITS ENTIRETY.
C

************************************************************

                  ***********************************
C                        'FORCE CONFIGURATION'
                  ***********************************

      DIMENSION VX(500),VY(500),VZ(500),PKE(500)
      DIMENSION DX(500),DY(500),DZ(500),PTE(500)
      DIMENSION PPESAV(500),PPEINT(500),PPEPOS(500),
     1PPENEG(500)
      DIMENSION FSTACC(100),FSSACC(100),FORMAX(100),
     1IFMXAM(100)
      DIMENSION DTFSP(50),DTIASP(50),DTESP(50),DTIVSP(50),
     1DETI(50)
      DIMENSION PPKEEP(500)
      DIMENSION DTSTEP(200)


                  ***********************************
C                       'OTHER CONFIGURATIONS'
                  ***********************************


      DIMENSION VX(500),VY(500),VZ(500),PKE(500)
      DIMENSION DX(500),DY(500),DZ(500),PTE(500)
      DIMENSION PPESAV(500),PPEINT(500),PPEPOS(500),
     1PPENEG(500)
      DIMENSION FSTACC(100),FSSACC(100),FORMAX(100),
     1IFMXAM(100)
      DIMENSION DT1(50),DT2(50),DT3(50),DT4(50)
      DIMENSION PPKEEP(500)
      DIMENSION DTSTEP(200)

************************************************************
```

```
C
C     PRESCRIBE COMMON STORAGE OF VARIABLES AND VARIABLE
C     ARRAYS REQUIRED IN SUBROUTINES.
C


      COMMON/COM1/RX(500),RY(500),RZ(500),LCUT(500),
     1LL,LD,ITYPE,NVAC
      COMMON/COM2/IH1(20),IH2(8),IHS(10),IHB(6),IHT(6),
     1TARGET(4),TMAS,BULLET(4),BMAS,PLANE,TEMP,THERM,
     1DDTII,DDTIF
      COMMON/COM3/RXI(500),RYI(500),RZI(500),CVR,EVR,
     1NT,TIME,DT,DTI,ILAY,RXK(500),RYK(500),RZK(500)
      COMMON/COM4/IX,IY,IZ,SCX,SCY,SCZ,IDEEP,D1X,D1Y,D1Z,
     1IVACX,IVACY,IVACZ
      COMMON/CCM5/ROE,ROE2,ROEM,EXA,EXB,PEXA,PEXB,FXA,PFXA,
     1IQ,TSAVE,BSAVE
      COMMON/COM6/FX(500),FY(500),FZ(500),PAC,PFPTC,FM
      COMMON/COM7/PPTC,TPOT,PPE(1000),TLPE,ROEL,ROEL2,NEW
      COMMON/COM8/ROEA,ROEB,ROEC,ROEC2,CP0,CP1,CP2,CP3,
     1CF0,CF1,CF2,CGD1,CGD2,CGB1,CGB2,CGF1,CGF2
      COMMON/COM9/XNVAC,YNVAC,ZNVAC
      COMMON/COM10/IXNEW,IYNEW,IZNEW,II
      COMMON/COM11/RXNEWI(250),RYNEWI(250),RZNEWI(250),
     1KEEP(250),NNUM(250)
      COMMON/COMA/ A(4,5),MCRO


C
C     LIST FORMAT STATEMENTS OF ALL READ COMMANDS.
C


 9010 FORMAT(20A4)
 9020 FORMAT(8A4,3F8.5,2F5.2)
 9030 FORMAT(4A4,3F8.5,6A4,F6.2)
 9040 FORMAT(F6.3,5X,I5,5I4,4X,3F5,3I2)
 9041 FORMAT(2F6.4,6F6.3)
 9042 FORMAT(F8.4,F8.4)
 9050 FORMAT(10A4,A4,4I3,F8.4,I4,F5.4)
 9052 FORMAT (6(F6.3))


C
C     LIST FORMAT STATEMENTS OF ALL WRITE COMMANDS.
C


 9610 FORMAT(1H1)
 9620 FORMAT(47X,'SUMMARY OF ATOMS'//,35X,8A4,', NT ='I4,//,
     13(' ATOM          POSITION           BIND ENERGY     '),//)
 9630 FORMAT(3(I5,3F6.2,F8.4,8X))
 9640 FORMAT(/4X,F10.3,25H EV,TOTAL KINETIC ENERGY,,F10.3,
     127H EV,TOTAL POTENTIAL ENERGY,F10.3,' EV, REDUCTION',/
     1/60X,'RADIUS =',F5.2,)
 9650 FORMAT(105X,4HPAGE,I3,/,1H1)
 9660 FORMAT(/  '        ATOM      DX          DY          DZ
     1VX          VY          VZ          KE          PE          TE',/)
 9670 FORMAT(1I8,3F10.3,3F10.1,3F10.4 )
 9680 FORMAT(' SHARP DT DECREASE',2E10.3)
 9690 FORMAT(I4,3F5.2,I4)
 9691 FORMAT(9F8.4)
 9692 FORMAT(1X,I4,/)
 9693 FORMAT(4(I5,3X,F8.4,9X))
 9694 FORMAT (22X,'SUMMARY OF POSITIVE POTENTIAL ENERGY CHAN
     1GES GREATER THAN',F7.4,2X,'NT=',I2,//,' ATOM     INITIA
     1L/FINAL X     INITIAL/FINAL Y     INITIAL/FINAL Z     PE
     1CHANGE'/)
 9695 FORMAT (22X,'SUMMARY OF NEGATIVE POTENTIAL ENERGY CHAN
     1GES GREATER THAN ',F7.4,2X,'NT=',I2,//,' ATOM     INITI
```

```
     1AL/FINAL X    INITIAL/FINAL Y    INITIAL/FINAL Z    PE
     1 CHANGE'/)
 9696 FORMAT (I5,7X,3(F6.2,13X),/,12X,2(F6.2,13X),F6.2,
     110X,F8.4)
 9697 FORMAT (10X,'INITIAL SUMMARY OF POTENTIAL ENERGY CHANG
     1ES ',//,(' ATOM  PE CHANGE         '))
 9699 FORMAT (40X,'FORCES AFTER EACH STEP',//,' STEP',10X,
     1'DT/STEP ',11X,'FMAX',9X,'ATOM WITH MAX FORCE',5X,
     1'FORCE (1)'/)
 9700 FORMAT (2X,I3,6X,E12.4,6X,E12.4,13X,I3,12X,E12.4)
 9704 FORMAT(20X,'DT CHECK FOR EACH STEP',//,'STEP',11X,
     1'STEP',11X,'DTE1',11X,'DTF1',11X,'DTE',11X,'DTF',//)
 9704 FORMAT(20X,'DT CHECK FOR EACH STEP',//,'STEP',11X,
     1'DTE1',11X,'DTF1',11X,'DTE',11X,'DTF',//)

**************************************************************

                 ************************************
C                       'FORCE CONFIGURATION'
                 ************************************


C
C     CHANGE STATEMENT NUMBER 9704 TO READ
C


 9704 FORMAT(20X,'DT CHECK FOR EACH STEP',//'STEP',11X,
     1'DTF',12X,'DTIA',11X,'DTE',11X,'DTIV',//)

**************************************************************

 9705 FORMAT(I5,4(3X,E12.4),/)

C
C     INITIALIZE APPROPRIATE VARIABLES AND VARIABLE ARRAYS.
C

      START=0.01*ITIME(XX)
      DO 2 I=1,1000
      RXK(I)=0.0
      RYK(I)=0.0
      RZK(I)=0.0
      VX(I)=0.0
      VY(I)=0.0
      VZ(I)=0.0
      PKE(I)=0.0
      PPE(I)=0.0
      PTE(I)=0.0
    2 RZI(I)=0.0
      ISHUT=1
      NRUN=0

C
C     READ INPUT DATA COMMON TO ALL DESIRED CALCULATIONS.
C

       READ ( 5,9010) IH1
       READ ( 5,9020) IH2,DCON,ALPHA,RE,ROEC,ROEL
       READ ( 5,9030) BULLET,BMAS,PEXA,PEXB,IHB,THERM
       READ ( 5,9030) TARGET,TMAS,EXA,EXB,IHT,TEMP
       READ ( 5,9050) IHS,PLANE,LS,IX,IY,IZ,CVR,MCRO ,DTI
      READ (5,9042) PPEPCK,PPENCK

C
C     INITIALIZE CONSTANTS AND DEFINE SCALING FACTORS.
C
```

```
      DTIS=DTI
      ROE2=4.0
      ROE=SQRT(ROE2)
      ROEM = ROE-DTI
      ROEL2=ROEL*ROEL
      CVE=1.60E-19
      CVM=1.672E-27
      VFAC=0.5
      FM=1.0E-10
      FM2=FM*FM
      CVD=CVR*1.0E-10
      CVED=CVE/CVD
      PTMAS=TMAS*CVM
      PBMAS=BMAS*CVM
      HTMAS=0.5*PTMAS/CVE
      HBMAS=0.5*PBMAS/CVE
      TSAVE=BMAS/(BMAS+TMAS)
      BSAVE=TMAS/(BMAS+TMAS)
C
C     DEFINE REPULSIVE POTENTIAL PARAMETERS.
C
      FXA=ALOG(-EXB*CVED)+EXA
      PFXA=ALOG(-PEXB*CVED)+PEXA
      PPTC=EXP(PEXA+PEXB*ROE)
      PAC=ALOG(CVED)+PEXA
      PFPTC=EXP(PAC+PEXB*ROE)
C
C     DEFINE ATTRACTIVE POTENTIAL PARAMETERS.
C
      CGD1=ALOG(DCON)+2.0*ALPHA*RE
      CGD2=ALOG(2.0*DCON)+ALPHA*RE
      CGB1=-2.0*ALPHA*CVR
      CGB2=-ALPHA*CVR
      CGF1=ALOG(-CGB1*CVED)+CGD1
      CGF2=ALOG(-CGB2*CVED)+CGD2
C
C     DEFINE REGIONS OF APPLICABILITY OF POTENTIAL FUNCTIONS
C
      ROEA=1.50/CVR
      ROEB=2.0/CVR
      ROEC2=ROEC*ROEC
C
C     DEFINE PARAMETERS USED TO DETERMINE THE BEST CUBIC
C     FIT BETWEEN THE MAXIMUM DISTANCE OF APPLICABILITY OF
C     OF THE REPULSIVE POTENTIAL AND THE MINIMUM DISTANCE
C     OF APPLICABILITY OF THE ATTRACTIVE POTENTIAL.
C     SUBROUTINE CROSYM PERFORMS THE NECESSARY CALCULATIONS.
C
      A(1,1)=1.0
      A(1,2)=ROEA
      A(1,3)=ROEA*ROEA
      A(1,4)=RCEA**3
      A(1,5)=EXP(EXA+EXB*ROEA)
      A(2,1)=1.0
```

```
      A(2,2)=ROEB
      A(2,3)=ROEB*ROEB
      A(2,4)=ROEB**3
      A(2,5)=EXP(CGD1+CGB1*ROEB)-EXP(CGD2+CGB2*ROEB)
      A(3,1)=0.0
      A(3,2)=-1.0
      A(3,3)=-2.0*ROEA
      A(3,4)=-3.0*ROEA*ROEA
      A(3,5)=EXP(EXA+EXB*ROEA)/CVED
      A(4,1)=0.0
      A(4,2)=-1.0
      A(4,3)=-2.0*ROEB
      A(4,4)=-3.0*ROEB*ROEB
      A(4,5)=(EXP(CGF1+CGB1*ROEB)-EXP(CGF2+CGB2*ROEB))/CVED
      CALL CROSYM
      CP0=A(1,5)
      CP1=A(2,5)
      CP2=A(3,5)
      CP3=A(4,5)
      CF0=-CP1*CVED
      CF1=-2.0*CP2*CVED
      CF2=-3.0*CP3*CVED


C
C     READ INPUT DATA FOR EACH SITE TO BE INVESTIGATED.
C     MULTIPLE INVESTIGATIONS ARE POSSIBLE BY SIMPLY READING
C     IN DATA FOR MORE THAN ONE SITE.
C


    5 READ ( 5,9040) EVR,NTT,NS,ND,IP,IDEEP,ITYPE, D1X,
     1D1Y,D1Z,IVACX,IVACY,IVACZ
      READ(5,9041,END=9999) DDTII,DDTIF,XNVAC,YNVAC,ZNVAC
************************************************************

            ************************************
C                  'FORCE CONFIGURATION'
            ************************************


C
C     IN THE FORCE CONFIGURATION ONLY, READ IN DTI VALUES
C     TO BE ASSIGNED AFTER FORCE COMPARISON, AND
C     DEFINE VARIABLE VFAC2.
C


      READ(5,9052) DTIA1,DTIA2,DTIA3,DTIV1,DTIV2,DTIV3
      VFAC2=VFAC*VFAC
************************************************************


      IF(NTT.EQ.0) GO TO 9999
      IQ=ITYPE-1
      EV=EVR*1.0E+3
      DTI=DTIS
      TPKE=EV

************************************************************

            ************************************
C              'POTENTIAL WELL CONFIGURATION'
            ************************************


C
C     CONSTRUCT A 'RELAXED' CRYSTAL IN THE COMPUTER BY
C     READING IN 'RELAXED' CRYSTAL PARAMETERS AND POSITIONS
```

```
C     VICE USING SUBROUTINE B100 TO CONSTRUCT THE CRYSTAL.
C


       READ  (5,9690) LL,D1X,D1Y,D1Z,NVAC
      DO 15 I=1,LL,3
      K=I+1
      J=I+2
       READ  (5,9691) RX(I),RY(I),RZ(I),RX(K),RY(K),RZ(K),
     1RX(J),RY(J),RZ(J)
   15 CONTINUE

                  ***********************************
C                       'OTHER CONFIGURATIONS'
                  ***********************************


C
C     SELECT THE DESIRED CRYSTAL STRUCTURE AND ORIENTATION.
C     SUBROUTINE B100 CONSTRUCTS THE (100) PLANES OF A BODY-
C     CENTERED CUBIC CRYSTAL IN THE COMPUTER.
C


   14 CALL B100
************************************************************


   30  ILAY=IDEEP
       IF(IDEEP) 35,35,40
   35 LD=LL
       ILAY=IY
   40 RLL=1.0/LL
      TPOTL=1.0
      DO 45 I=1,LL
      RXK(I)=RX(I)
      RYK(I)=RY(I)
      RZK(I)=RZ(I)
      RXI(I)=RX(I)
      RYI(I)=RY(I)
   45 RZI(I)=RZ(I)
C
      IF(NRUN.EQ.0) GO TO 60
      DO 55 I=1,LL
      LCUT(I)=0
      RX(I)=RXI(I)
      RY(I)=RYI(I)
      RZ(I)=RZI(I)
      RXK(I)=RXI(I)
      RYK(I)=RYI(I)
   55 RZK(I)=RZI(I)
   60 NRUN=1


C
C     THIS SECTION CALCULATES THE ENERGIES OF ALL ATOMS IN
C     THEIR INITIAL POSITIONS IN THE PERFECT LATTICE (THAT
C     IS, WITH NO INTERSTITIAL IMPLANTED). INITIAL POSITIONS
C     AND ENERGIES OF ALL ATOMS ARE PRINTED TO PROVIDE A
C     COMPARISON WITH CHANGES IN CRYSTAL ATOM POSITIONS
C     AND ENERGIES CAUSED BY IMPLANTATION OF THE INTERSTI-
C     TIAL.
C

************************************************************

                  ***********************************
C                   'POTENTIAL WELL CONFIGURATION'
                  ***********************************
```

```
C
C      THIS CALCULATION CAN NOT BE MADE IN THE POTENTIAL
C      WELL CONFIGURATION WITHOUT DESTROYING THE INPUT
C      DATA OF THE 'RELAXED' CRYSTAL. CONSEQUENTLY,
C
C                          RX(1)=25.0
C
C      SHOULD BE DELETED IN THE POTENTIAL WELL CONFIGURATION.
C
***************************************************************


      RX(1)=25.0
      DO 63 I=1,LL
      VX(I)=0.0
      VY(I)=0.0
      VZ(I)=0.0
      PPE(I)=0.0
      PKE(I)=0.0
   63 PTE(I)=0.0
      TPOT=0.0
      NEW=0
      CALL ENERGY
      NPAGE=1
      NT=0
       WRITE ( 6,9610)
       WRITE ( 6,9620) IH2,NT
      DO 61 I=1,LL,3
      K=I+1
      J=I+2
   61  WRITE ( 6,9630) I,RX(I),RY(I),RZ(I),PPE(I),K,RX(K),
     1RY(K),RZ(K),PPE(K),J,RX(J),RY(J),RZ(J),PPE(J)
       WRITE ( 6,9650) NPAGE
      DO 62 I=1,LL,3
      K=I+1
      J=I+2
      PPESAV(I)=PPE(I)
      PPESAV(K)=PPE(K)
      PPESAV(J)=PPE(J)
   62 CONTINUE

***************************************************************

                   ***********************************
C                   'POTENTIAL WELL CONFIGURATION'
                   ***********************************


C
C      THE VARIABLES BELOW ARE USED TO CREATE OFFSETS FROM
C      EQUILIBRIUM POSITIONS IN THE 'RELAXED' CRYSTAL. IF
C      NO OFFSET IS DESIRED, THESE VARIABLES SHOULD BE
C      INCLUDED BUT SET EQUAL TO ZERO. THE OFFSET IS
C      INSTITUTED BY SUBROUTINE PLACE. THESE VARIABLES
C      SHOULD NOT BE INCLUDED IN OTHER CONFIGURATIONS.
C


      D1X=0.0
      D1Y=0.0
      D1Z=0.0

***************************************************************


C
C      SUBROUTINE PLACE CREATES THE DESIRED VACANCY, INTER-
C      STITIAL, OR SELF INTERSTITIAL IN THE CRYSTAL.
C      IN THE POTENTIAL WELL CONFIGURATION, THE INTERSTITIAL
```

```
C      IS OFFSET FROM ITS EQUILIBRIUM POSITION.
C


       CALL PLACE
       DO 65 I=1,LL
       VX(I)=0.0
       VY(I)=0.0
       VZ(I)=0.0
       PPE(I)=0.0
       PKE(I)=0.0
    65 PTE(I)=0.0
       TPOT=0.0
       NEW=0


C
C      THE ENERGY SUBROUTINE NOW CALCULATES ENERGIES OF ALL
C      ATOMS OF THE CRYSTAL AFTER IMPLANTATION. THESE
C      ENERGIES AND THE INITIAL POSITIONS OF ALL ATOMS ARE
C      PRINTED FOR TIME ZERO. CHANGES IN POTENTIAL ENERGY OF
C      ALL ATOMS AS A RESULT OF IMPLANTATION ARE ALSO CALCU-
C      LATED AND PRINTED.
C


       CALL ENERGY
       BIND=-TPOT
       TE=TPOT+BIND
C
       TIME=0.0
       NT=0
        WRITE ( 6,9620) IH2,NT
       DO 70 I=1,LL,3
       K=I+1
       J=I+2
    70  WRITE ( 6,9630) I,RX(I),RY(I),RZ(I),PPE(I),K,RX(K),
      1RY(K),RZ(K),PPE(K),J,RX(J),RY(J),RZ(J),PPE(J)
        WRITE ( 6,9640) TPKE,TPOT,TE,ROEL
       NPAGE=NPAGE+1
        WRITE ( 6,9650) NPAGE
       WRITE (6,9697)
       DO 80 I=1,LL,4
       K=I+1
       J=I+2
       L=I+3
       PPEINT(I)=PPE(I)-PPESAV(I)
       PPEINT(K)=PPE(K)-PPESAV(K)
       PPEINT(J)=PPE(J)-PPESAV(J)
       PPEINT(L)=PPE(L)-PPESAV(L)
    80 WRITE (6,9693) I,PPEINT(I),K,PPEINT(K),J,PPEINT(J),L,
      1PPEINT(L)
       NPAGE=NPAGE+1
       WRITE (6,9650) NPAGE
       DT=1.0E-15

*************************************************************************

                 ************************************
C                         'FORCE CONFIGURATION'
                 ************************************


C
C      SINCE TIMESTEPS IN THIS CONFIGURATION ARE DETERMINED
C      DIRECTLY BY A FORCE COMPARISON, NO TIMESTEP
C      DECREMENTING PROCEDURE IS REQUIRED. THE ONLY CARD
C      NEEDED IS

   100 CONTINUE
```

```
                **********************************
C                    'OTHER CONFIGURATIONS'
                **********************************


C
C     THE FOLLOWING STATEMENTS DEFINE THE DTI
C     DECREMENTING PROCEDURE.
C


      DDTI=DDTII
      NDEC=0
  100 DTI=DTI-DDTI
      IF(DTI.LT.DDTIF) DTI=DDTIF
  105 NDEC=NDEC+1
*****************************************************************


C
C     THE MAIN BODY OF THE PROGRAM NOW SOLVES THE EQUATIONS
C     OF MOTION BY THE AVERAGE FORCE METHOD AND DETERMINES
C     POSITIONS OF ALL ATOMS AT THE END OF THIS TIMESTEP.
C     SUBROUTINE STEP PERFORMS ALL FORCE CALCULATIONS.
C


      DTOD=DT/CVD
      TFAC=2.0*PTMAS*DTI*CVD
      TFACB=2.0*PBMAS*DTI*CVD
      TEFAC=DTI*CVD
      HDTOD=0.5*DTOD
      DTOM=DT/PTMAS
      HDTOM=0.5*DTOM
      DTOMB=DT/PBMAS
      HDTOMB=0.5*DTOMB
  200 CALL STEP
      IF(LCUT(1).GT.0) GO TO 240
      I=1
      RXK(I)=RX(I)
      RYK(I)=RY(I)
      RZK(I)=RZ(I)
      RX(I)=RX(I)+DTOD*(HDTOMB*FX(I)+VX(I))
      RY(I)=RY(I)+DTOD*(HDTOMB*FY(I)+VY(I))
      RZ(I)=RZ(I)+DTOD*(HDTOMB*FZ(I)+VZ(I))
  240 DO 245 I=2,LD
      IF(LCUT(I).GT.0)GO TO 245
      RXK(I)=RX(I)
      RYK(I)=RY(I)
      RZK(I)=RZ(I)
      RX(I)=RX(I)+DTOD*(HDTOM*FX(I)+VX(I))
      RY(I)=RY(I)+DTOD*(HDTOM*FY(I)+VY(I))
      RZ(I)=RZ(I)+DTOD*(HDTOM*FZ(I)+VZ(I))
  245 CONTINUE
      CALL STEP
      FSTACC(NT)=SQRT(FX(1)**2+FY(1)**2+FZ(1)**2)/BMAS
      EMAX=0.0
      FMAX=0.0
      TIME=TIME+DT
      NT=NT+1
      IF(LCUT(1).GT.0) GO TO 265
      I=1
      VSS=VX(I)
      VX(I)=VSS+HDTOMB*FX(I)
      RX(I)=RXK(I)+(VX(I)+VSS)*HDTOD
      VSS=VY(I)
      VY(I)=VSS+HDTOMB*FY(I)
      RY(I)=RYK(I)+(VY(I)+VSS)*HDTOD
      VSS=VZ(I)
```

```
      VZ(I)=VSS+HDTOMB*FZ(I)
      RZ(I)=RZK(I)+(VZ(I)+VSS)*HDTOD
      PKE(I)=VX(I)*VX(I)+VY(I)*VY(I)+VZ(I)*VZ(I)
      EMAX1=PKE(I)
      FMAX12=FX(I)*FX(I)+FY(I)*FY(I)+FZ(I)*FZ(I)
      FMAX1=SQRT(FMAX12)
      AMAX1=FMAX1/BMAS
      FSSACC(NT)=AMAX1
  260 FX(I)=0.0
      FY(I)=0.0
      FZ(I)=0.0
      FMAX=0.0
      EMAX=0.0
      F2M=0.0
  265 DO 280 I=2,LD
      IF(LCUT(I).GT.0)GO TO 280
      VSS=VX(I)
      VX(I)=VSS+HDTOM*FX(I)
      RX(I)=RXK(I)+(VX(I)+VSS)*HDTOD
      VSS=VY(I)
      VY(I)=VSS+HDTOM*FY(I)
      RY(I)=RYK(I)+(VY(I)+VSS)*HDTOD
      VSS=VZ(I)
      VZ(I)=VSS+HDTOM*FZ(I)
      RZ(I)=RZK(I)+(VZ(I)+VSS)*HDTOD
      PKE(I)=VX(I)*VX(I)+VY(I)*VY(I)+VZ(I)*VZ(I)
  275 F2=FX(I)*FX(I)+FY(I)*FY(I)+FZ(I)*FZ(I)
      FX(I)=0.0
      FY(I)=0.0
      FZ(I)=0.0
      IF(F2.LE.F2M) GO TO 278
      F2M=F2
      IFMXAM(NT)=I
  278 IF(PKE(I).GT.EMAX) EMAX=PKE(I)
  280 CONTINUE
      FMAX=SQRT(F2M)
      AMAXL=FMAX/TMAS
      FORMAX(NT)=AMAXL

************************************************************

             ***********************************
C                   'FORCE CONFIGURATION'
             ***********************************


C
C     TIMESTEP DETERMINATION IN THE FORCE CONFIGURATION
C     IS PERFORMED BY COMPARING THE MAXIMUM FORCE IN THE
C     CRYSTAL WITH APPROPRIATELY CHOSEN TEST VALUES.
C


      AMAX=AMAX1
      IF(AMAXL.GT.AMAX) GO TO 282
      IFMXAM(NT)=1
      GO TO 284
  282 AMAX=AMAXL
  284 DTL=DT
      EMAXL=EMAX*VFAC2
      IF(AMAX.LE.1.0E-8) DTIA=DTIA1
      IF(AMAX.LE.1.0E-9) DTIA=DTIA2
      IF(AMAX.LE.1.0E-10) DTIA=DTIA3
      IF(AMAX.LE.1.0E-11) ISHUT=-1
      CTIME=0.01*ITIME(XX)-START
      EMAX=EMAX1
      IF(EMAXL.GT.EMAX) EMAX=EMAXL
      IF(EMAX.LE.1.0E+6) DTIV=DTIV1
      IF(EMAX.LE.1.0E+4) DTIV=DTIV2
      IF(EMAX.LE.1.0E+2) DTIV=DTIV3
      DTFCK=(DTIA*CVD*2.0)/(AMAX/CVM)
```

```
      IF(DTFCK.LT.0.0)DTFCK=-DTFCK
      DTF=SQRT(DTFCK)
      DTFSP(NT)=DTF
      DTIASP(NT)=DTIA
      IF(EMAX.GT.0.0) GO TO 290
      DTE=1.0E-5
      GO TO 295
  290 DTE=(DTIV*CVD)/SQRT(EMAX)
  295 DTESP(NT)=DTE
      DTIVSP(NT)=DTIV
      DT=DTF
      IF(DTE.LE.DT)DT=DTE
      DTSTEP(NT)=DT

             ***********************************
C                  'OTHER CONFIGURATIONS'
             ***********************************


C
C     FOUR NEW TIMESTEPS ARE CALCULATED BASED ON MAXIMUM
C     FORCES AND ENERGIES OF INITIAL AND FINAL POSITIONS.
C     THE SMALLEST IS CHOSEN AS THE NEXT TIMESTEP INTERVAL.
C


      DTL=DT
      CTIME=0.01*ITIME(XX)-START
      DTE1=TEFAC*SQRT(1.0/EMAX1)
      DTF1=SQRT(TFACB/FMAX1)
      DTE=TEFAC*SQRT(1.0/EMAX)
      DTF=SQRT(TFAC/FMAX)
      DT1(NT)=DTE1
      DT2(NT)=DTF1
      DT3(NT)=DTE
      DT4(NT)=DTF
      IF(EMAX1.GT.EMAX) EMAX=EMAX1
      DT=DTE1
      IF(DT.GT.DTF1) DT=DTF1
      IF(DT.GT.DTE) DT=DTE
      IF(DT.GT.DTF) DT=DTF
      DTSTEP(NT)=DT
************************************************************


C
C     DAMPING IS INTRODUCED IN THE FORM OF A DAMPING FACTOR
C     WHICH DECREMENTS ALL VELOCITY COMPONENTS.
C


  300 IF(ISHUT.EQ.-1) GO TO 400
  310 IF(NS-NT) 400,400,320
  320 DO 325 I=1,LL
      VX(I)=VFAC*VX(I)
      VY(I)=VFAC*VY(I)
  325 VZ(I)=VFAC*VZ(I)

************************************************************

             ***********************************
C                   'FORCE CONFIGURATION'
             ***********************************


C
C     SINCE THE TIMESTEP HAS ALREADY BEEN DETERMINED IN THE
C     FORCE METHOD, THE COMPUTATION CAN NOW SHIFT TO
C     STATEMENT NUMBER 100 AND BEGIN THE DYNAMICS FOR THE
```

```
C     NEXT TIMESTEP.
C

      GO TO 100

             ***********************************
C                  'OTHER CONFIGURATIONS'
             ***********************************

C
C     SHIFT TO STATEMENT NUMBER 800 FOR CALCULATION OF THE
C     DTI DECREMENT IF REQUIRED FOR THIS TIMESTEP.
C

      GO TO 800
************************************************************

C
C     SUBROUTINE PRINT PRINTS PERTINENT GENERAL DATA FOR
C     EACH TIMESTEP PRINTOUT.
C

  400 CALL PRINT

C
C     RELATIVE MOTION, VELOCITY, AND ENERGY OF EACH ATOM
C     ARE PERIODICALLY PRINTED.
C

  410 TPOT=0.0
      DO 450 I=1,LL
      PPE(I)=0.0
  450 PTE(I)=0.0
      CALL ENERGY
      PKE(1)=HBMAS*PKE(1)
      TPKE=PKE(1)
      PTE(1)=PKE(1)+PPE(1)
      DO 620 I=2,LL
      PKE(I)=HTMAS*PKE(I)
      TPKE=TPKE+PKE(I)
  620 PTE(I)=PKE(I)+PPE(I)
      TE=TPOT+BIND
       WRITE ( 6,9660)
      DTEST=0.1*(RX(1)-RXI(1))**2
      IF (DTEST.GT. 0.01) DTEST= 0.01
      IF(TPOT.LE.TPOTL) GO TO 700
      ERAT=TPKE*RLL
  700 DO 750 I=1,LD
      DX(I)=RX(I)-RXI(I)
      DY(I)=RY(I)-RYI(I)
      DZ(I)=RZ(I)-RZI(I)
      IF (DX(I)**2.GE.DTEST) GO TO 720
      IF (DY(I)**2.GE.DTEST) GO TO 720
      IF (DZ(I)**2.GE.DTEST) GO TO 720
      GO TO 750
C
  720  WRITE ( 6,9670) I,DX(I),DY(I),DZ(I),VX(I),VY(I),
     1VZ(I),PKE(I),PPE(I),PTE(I)
  750 CONTINUE
       WRITE ( 6,9640) TPKE,TPOT,TE,ROEL
      NPAGE=NPAGE+1
       WRITE ( 6,9650) NPAGE
      TPOTL=TPOT
```

```
      IF(NT-NTT) 760,950,950
  760 DO 780 I=1,LL
      VX(I)=VFAC*VX(I)
      VY(I)=VFAC*VY(I)
      VZ(I)=VFAC*VZ(I)
  780 CONTINUE
      IF(ISHUT.EQ.-1) GO TO 950
  790 NS=NS+ND

****************************************************************

                 ***********************************
C                       'FORCE CONFIGURATION'
                 ***********************************


C
C     NO DECREMENTING PROCEDURE FOR DTI IS NEEDED, SO THE
C     FORCE CONFIGURATION SHIFTS TO STATEMENT NUMBER 100
C     AND BEGINS COMPUTATIONS FOR THE NEXT TIMESTEP.
C


  830 GO TO 100

                 ***********************************
C                      'OTHER CONFIGURATIONS'
                 ***********************************


C
C     THE DTI ALTERATION PROCESS IS BEGUN FOR THE NEXT
C     TIMESTEP
C


  800 IF(NDEC.EQ.10) GO TO 810
      GO TO 820
  810 DDTI=0.1*DDTI
      DTI=DTI+DDTI
      NDEC=0
  820 GO TO 100
****************************************************************


  950 CONTINUE


C
C     FINAL POSITIONS (IN RECTANGULAR COORDINATES) AND
C     BINDING ENERGIES OF ALL ATOMS ARE PRINTED AFTER THE
C     LAST TIMESTEP. WRITE (7,XXXX) STATEMENTS ARE INCLUDED
C     WHEN DATA DECKS CONTAINING COMPLETE INFORMATION FOR
C     THE ENTIRE CRYSTAL ARE DESIRED. ADDITIONALLY, POSITIVE
C     AND NEGATIVE POTENTIAL ENERGY CHANGES GREATER THAN
C     A PRESET VALUE ARE DETERMINED AND PRINTED.
C


  955  WRITE ( 6,9620) IH2,NT
      WRITE (7,9690) LL,D1X,D1Y,D1Z,NVAC
      DO 965 I=1,LL,3
      K=I+1
      J=I+2
      WRITE (7,9691) RX(I),RY(I),RZ(I),RX(K),RY(K),RZ(K),
     1RX(J),RY(J),RZ(J)
  965  WRITE ( 6,9630) I,RX(I),RY(I),RZ(I),PPE(I),K,RX(K),
     1RY(K),RZ(K),PPE(K),J,RX(J),RY(J),RZ(J),PPE(J)
       WRITE ( 6,9640) TPKE,TPOT,TE,ROEL
```

```
      NPAGE=NPAGE+1
       WRITE ( 6,9650) NPAGE
      DO 970 I=1,LL
      PPEPOS(I)=0.0
      PPENEG(I)=0.0
      PPKEEP(I)=PPE(I)-PPESAV(I)
      IF(PPKEEP(I).GT.PPEPCK) GO TO 968
      IF(PPKEEP(I).GT.PPENCK) GO TO 970
      PPENEG(I)=PPKEEP(I)
      GO TO 970
  968 PPEPOS(I)=PPKEEP(I)
  970 CONTINUE
      WRITE (6,9694) PPEPCK,NT
      DO 980 I=1,LL
      IF(PPEPOS(I).LT.PPEPCK) GO TO 980
      WRITE (6,9696) I,RXI(I),RYI(I),RZI(I),RX(I),RY(I),
     1RZ(I),PPEPOS(I)
  980 CONTINUE
      NPAGE=NPAGE+1
      WRITE (6,9650) NPAGE
      WRITE(6,9695)PPENCK,NT
      DO 990 I=1,LL
      IF(PPENEG(I).GT.PPENCK) GO TO 990
       WRITE (6,9696) I,RXI(I),RYI(I),RZI(I),RX(I),RY(I)
     1RZ(I),PPENEG(I)
  990 CONTINUE
      NPAGE=NPAGE+1
      WRITE (6,9650) NPAGE
      WRITE (6,9699)
      DO 995 I=1,NT
  995 WRITE (6,9700) I,DTSTEP(I),FORMAX(I),IFMXAM(I),
     1FSSACC(I)
      NPAGE=NPAGE+1
      WRITE (6,9650) NPAGE
      WRITE (6,9704)
      DO 999 I=1,NT

************************************************************

             ************************************
C                  'FORCE CONFIGURATION'
             ************************************


C
C     DATA PERTINENT TO TIMESTEP DETERMINATION BY THE
C     FORCE METHOD ARE PRINTED.
C


  999 WRITE (6,9705) I,DTFSP(I),DTIASP(I),DTESP(I),DTIVSP(I)


             ************************************
C                 'OTHER CONFIGURATIONS'
             ************************************


C
C     DATA PERTINENT TO TIMESTEP DETERMINATION BY THE
C     ENERGY METHOD ARE PRINTED.
C


  999 WRITE (6,9705) I,DT1(I),DT2(I),DT3(I),DT4(I)
************************************************************


************************************************************
```

```
                  **********************************
C                        'PLUCK CONFIGURATION'
                  **********************************


C
C      SUBROUTINE PLUCK CAN BE USED TO  PUNCH DATA CARDS FOR
C      A SMALLER CRYSTAL CENTERED ON THE INTERSTITIAL FOR
C      USE IN THE DYNAMIC PROGRAM. DELETE THESE CARDS IF
C      DATA FOR THE SMALLER CRYSTAL IS NOT DESIRED
C


      CALL PLUCK
      WRITE (7,9690) LL,D1X,D1Y,D1Z,NVAC,IXNEW,IYNEW,IZNEW
      LL=II
      DO 1100 I=1,LL
 1100 WRITE (7,9691) I,RXNEWI(I),RYNEWI(I),RZNEWI(I),KEEP(I)
**************************************************************


 1000 IF(ISHUT) 9999,5,5
 9999 STOP
      END


C
C      SUBROUTINE CROYSM SOLVES M SIMULTANEOUS EQUATIONS BY
C      THE METHOD OF CROUT IN ORDER TO FIT THE BEST CUBIC
C      EQUATION BETWEEN THE REPULSIVE AND ATTRACTIVE PARTS
C      OF THE POTENTIAL.
C


      SUBROUTINE CROSYM
C
C
      COMMON/COMA/ A(4,5),MCRO
      M=MCRO
      N=M+1
      I1=1
  100 I3=I1
      SUM=ABS(A(I1,I1))
      DO 120 I=I1,M
      IF(SUM-ABS(A(I,I1))) 110,120,120
  110 I3=I
      SUM=ABS(A(I,I1))
  120 CONTINUE
      IF(I3-I1) 130,150,130
  130 DO 140 J=1,N
      SUM=-A(I1,J)
      A(I1,J)=A(I3,J)
  140 A(I3,J)=SUM
  150 I3=I1+1
      DO 160 I=I3,M
  160 A(I,I1)=A(I,I1)/A(I1,I1)
  170 J2=I1-1
      I3=I1+1
      IF(J2) 180,200,180
  180 DO 190 J=I3,N
      DO 190 I=1,J2
  190 A(I1,J)=A(I1,J)-A(I1,I)*A(I,J)
      IF(I1-M) 200,220,200
  200 J2=I1
      I1=I1+1
      DO 210 I=I1,M
      DO 210 J=1,J2
  210 A(I,I1)=A(I,I1)-A(I,J)*A(J,I1)
      IF(I1-M) 100,170,100
```

```
  220 DO 240 I=1,M
      J2=M-I
      I3=J2+1
      A(I3,N)=A(I3,N)/A(I3,I3)
      IF(J2) 230,250,230
  230 DO 240 J=1,J2
  240 A(J,N)=A(J,N)-A(I3,N)*A(J,I3)
  250 RETURN
      END
C
C     SUBROUTINE B100 GENERATES A BODY-CENTERED CUBIC
C     LATTICE IN THE (100) DIRECTION.
C
C


      SUBROUTINE B100
C


      COMMON/COM1/RX(500),RY(500),RZ(500),LCUT(500),
     1LL,LD,ITYPE,NVAC
      COMMON/COM4/IX,IY,IZ,SCX,SCY,SCZ,IDEEP,D1X,D1Y,
     1D1Z,IVACX,IVACY,IVACZ
      DIMENSION YLAX(20)
      DATA YLAX/20*0.0/
      YLAX(1)=-0.20
      YLAX(2)=-0.03
      SCX=1.0
      SCY=1.0
      SCZ=1.0
      M = 2
      JT=0
      Y=-SCY
      DO 60 J=1,IY
      Y=Y+SCY
      KT=0
      Z=-SCZ
      DO 59 K=1,IZ
      Z=Z+SCZ
      IT=0
      X=-SCX
      DO 58 I=1,IX
      X=X+SCX
      IF(IT-(IT/2)*2) 21,11,21
   11 IF(JT-(JT/2)*2) 57,12,57
   12 IF(KT-(KT/2)*2) 57,30,57
   21 IF(JT-(JT/2)*2) 22,57,22
   22 IF(KT-(KT/2)*2) 30,57,30
   30 RX(M)=X
      RY(M)=Y+YLAX(J)
      RZ(M)=Z
      M=M+1
      IF (IT.NE.IVACX) GO TO 57
      IF (JT.NE.IVACY) GO TO 57
      IF (KT.NE.IVACZ) GO TO 57
      NVAC=M-1
   57 IT=IT+1
   58 CONTINUE
      KT=KT+1
   59 CONTINUE
      JT = JT + 1
      IF(IDEEP-JT) 60,110,60
   60 CONTINUE
      LL=M-1
  100 RETURN
  110 LD=M-1
      GO TO 60
      END
```

```
*****************************************************************************

                *********************************
C                 'POTENTIAL WELL CONFIGURATION'
                *********************************


C
C     SUBROUTINE PLACE OFFSETS THE INTERSTITIAL IN THE
C     'RELAXED' CRYSTAL.
C



      SUBROUTINE PLACE
C
C
      COMMON/COM1/RX(500),RY(500),RZ(500),LCUT(500),
     1LL,LD,ITYPE,NVAC
      COMMON/COM3/RXI(500),RYI(500),RZI(500),CVR,EVR,
     1NT,TIME,DT,DTI,ILAY,RXK(500),RYK(500),RZK(500)
      COMMON/COM4/IX,IY,IZ,SCX,SCY,SCZ,IDEEP,D1X,D1Y,
     1D1Z,IVACX,IVACY,IVACZ
      COMMON/COM9/XNVAC,YNVAC,ZNVAC
      GO TO  (10,20,30,40), ITYPE
   10 LCUT(NVAC) = 1
      LCUT(1) = 1
      RX(1)=0.0
      RY(1)=0.0
      RZ(1)=0.0
      GO TO 50
   20 RX(1)=RX(1)+D1X
      RY(1)=RY(1)+D1Y
      RZ(1)=RZ(1)+D1Z
      GO TO 50
   30 LCUT(NVAC)  = 1
      RX(1)  =  RX(NVAC)
      RY(1)  =  RY(NVAC)
      RZ(1)  =  RZ(NVAC)
      GO TO 50
   40 RX(1)=RX(1)+D1X
      RY(1)=RY(1)+D1Y
      RZ(1)=RZ(1)+D1Z
   50 CONTINUE
      RX(NVAC)=RX(NVAC)+XNVAC
      RY(NVAC)=RY(NVAC)+YNVAC
      RZ(NVAC)=RZ(NVAC)+ZNVAC
      RXI(NVAC)=RX(NVAC)
      RYI(NVAC)=RY(NVAC)
      RZI(NVAC)=RZ(NVAC)
      RXK(NVAC)=RX(NVAC)
      RYK(NVAC)=RY(NVAC)
      RZK(NVAC)=RZ(NVAC)
      RXI(1)=RX(1)
      RYI(1)=RY(1)
      RZI(1)=RZ(1)
      RXK(1)=RX(1)
      RYK(1)=RY(1)
      RZK(1)=RZ(1)
      RETURN
      END

                **********************************
C                    'OTHER CONFIGURATIONS'
                **********************************

C
C     SUBROUTINE PLACE CREATES A VACANCY OR IMPLANTS AN
```

```
C     INTERSTITIAL OR SELF INTERSTITIAL IN THE LATTICE.
C     LATTICE ATOMS ARE ALSO OFFSET AS REQUIRED BY
C     INPUT DATA.
C



      SUBROUTINE PLACE
C
C
      COMMON/COM1/RX(500),RY(500),RZ(500),LCUT(500),
     1LL,LD,ITYPE,NVAC
      COMMON/COM3/RXI(500),RYI(500),RZI(500),CVR,EVR,
     1NT,TIME,DT,DTI,ILAY,RXK(500),RYK(500),RZK(500)
      COMMON/COM4/IX,IY,IZ,SCX,SCY,SCZ,IDEEP,D1X,D1Y,
     1D1Z,IVACX,IVACY,IVACZ
      COMMON/COM9/XNVAC,YNVAC,ZNVAC
      GO TO  (10,20,30,40), ITYPE
   10 LCUT(NVAC) = 1
      LCUT(1) = 1
      RX(1)=0.0
      RY(1)=0.0
      RZ(1)=0.0
      GO TO 50
   20 RX(1)=RX(NVAC)+D1X
      RY(1)=RY(NVAC)+D1Y
      RZ(1)=RZ(NVAC)+D1Z
      GO TO 50
   30 LCUT(NVAC) = 1
      RX(1)  =  RX(NVAC)
      RY(1)  =  RY(NVAC)
      RZ(1)  =  RZ(NVAC)
      GO TO 50
   40 RX(1)=RX(NVAC)+D1X
      RY(1)=RY(NVAC)+D1Y
      RZ(1)=RZ(NVAC)+D1Z
   50 CONTINUE
      RX(NVAC)=RX(NVAC)+XNVAC
      RY(NVAC)=RY(NVAC)+YNVAC
      RZ(NVAC)=RZ(NVAC)+ZNVAC
      RXI(NVAC)=RX(NVAC)
      RYI(NVAC)=RY(NVAC)
      RZI(NVAC)=RZ(NVAC)
      RXK(NVAC)=RX(NVAC)
      RYK(NVAC)=RY(NVAC)
      RZK(NVAC)=RZ(NVAC)
      RXI(1)=RX(1)
      RYI(1)=RY(1)
      RZI(1)=RZ(1)
      RXK(1)=RX(1)
      RYK(1)=RY(1)
      RZK(1)=RZ(1)
      RETURN
      END
************************************************************

C
C     SUBROUTINE STEP CALCULATES FORCES ON THE INTERSTITIAL
C     AND ALL OTHER ATOMS OF THE CRYSTAL.
C
C


      SUBROUTINE STEP
C

C
      COMMON/COM1/RX(500),RY(500),RZ(500),LCUT(500),
```

```
     1LL,LD,ITYPE,NVAC
      COMMON/COM5/ROE,ROE2,ROEM,EXA,EXB,PEXA,PEXB,FXA,PFXA,
     1IQ,TSAVE,BSAVE
      COMMON/COM6/FX(500),FY(500),FZ(500),PAC,PFPTC,FM
      COMMON/COM8/ROEA,ROEB,ROEC,ROEC2,CP0,CP1,CP2,CP3,
     1CF0,CF1,CF2,CGD1,CGD2,CGB1,CGB2,CGF1,CGF2
      IF (IQ-1) 100,101,102
  100 IP=2
      GO TO 200
  101 IP=1
      GO TO 200
  102 I=1
      IP=2
  105 DO 195 J=IP,LL
      IF(LCUT(J)) 195,110,195
  110 DRX=RX(J)-RX(I)
      IF(DRX) 113,117,117
  113 IF(DRX+ROE) 195,195,120
  117 IF(DRX-ROE) 120,195,195
  120 DRY=RY(J)-RY(I)
      IF(DRY) 123,127,127
  123 IF(DRY+ROE) 195,195,130
  127 IF(DRY-ROE) 130,195,195
  130 DRZ=RZ(J)-RZ(I)
      IF(DRZ) 133,137,137
  133 IF(DRZ+ROE) 195,195,140
  137 IF(DRZ-ROE) 140,195,195
  140 DIST=DRX*DRX+DRY*DRY+DRZ*DRZ
       IF(DIST-ROE2) 150,195,195
  150 DIST=SQRT(DIST)
  160 IF(DIST-ROEM) 162,162,165
  162 FORCE=EXP(PFXA+PEXB*DIST)
      GO TO 180
  165 DFF=ROE-DIST
       IF(DFF-1.0E-10) 195,195,167
  167 FORCE=(EXP(PAC+PEXB*DIST)-PFPTC)/DFF
  180 IF(FM-FORCE) 190,190,195
  190 FOD=FORCE/DIST
      FA=FOD*DRX
      FX(J)=FX(J)+FA
      FX(I)=FX(I)-FA
      FA=FOD*DRY
      FY(J)=FY(J)+FA
      FY(I)=FY(I)-FA
      FA=FOD*DRZ
      FZ(J)=FZ(J)+FA
      FZ(I)=FZ(I)-FA
  195 CONTINUE
C
  200 DO 300 I=IP,LD
      IF(LCUT(I)) 300,205,300
  205 IP=I+1
      DO 295 J=IP,LL
      IF(LCUT(J)) 295,210,295
  210 DRX=RX(J)-RX(I)
      IF(DRX) 213,217,217
  213 IF(DRX+ROEC) 295,295,220
  217 IF(DRX-ROEC) 220,295,295
  220 DRY=RY(J)-RY(I)
      IF(DRY) 223,227,227
  223 IF(DRY+ROEC) 295,295,230
  227 IF(DRY-ROEC) 230,295,295
  230 DRZ=RZ(J)-RZ(I)
      IF(DRZ) 233,237,237
  233 IF(DRZ+ROEC) 295,295,240
  237 IF(DRZ-ROEC) 240,295,295
  240 DIST=DRX*DRX+DRY*DRY+DRZ*DRZ
       IF(DIST-ROEC2) 250,295,295
  250 DIST=SQRT(DIST)
       IF(DIST-ROEA) 260,255,255
  255 IF(DIST-ROEB) 265,270,270
  260 FORCE=EXP(FXA+EXB*DIST)
```

```
      GO TO 280
  265 FORCE=DIST*(DIST*CF2+CF1)+CF0
      GO TO 280
  270 FORCE=EXP(CGF1+CGB1*DIST)-EXP(CGF2+CGB2*DIST)
  280 FOD=FORCE/DIST
      FA=FOD*DRX
      FX(J)=FX(J)+FA
      FX(I)=FX(I)-FA
      FA=FOD*DRY
      FY(J)=FY(J)+FA
      FY(I)=FY(I)-FA
      FA=FOD*DRZ
      FZ(J)=FZ(J)+FA
      FZ(I)=FZ(I)-FA
  295 CONTINUE
  300 CONTINUE
      RETURN
      END


C
C     SUBROUTINE ENERGY CALCULATES MUTUAL POTENTIAL ENERGIES
C     FOR THE INTERSTITIAL AND ALL OTHER ATOMS OF THE
C     CRYSTAL.
C


C


      SUBROUTINE ENERGY
C
C
      COMMON/COM1/RX(500),RY(500),RZ(500),LCUT(500),
     1LL,LD,ITYPE,NVAC
      COMMON/COM5/ROE,ROE2,ROEM,EXA,EXB,PEXA,PEXB,FXA,PFXA,
     1IQ,TSAVE,BSAVE
      COMMON/COM7/PPTC,TPOT,PPE(1000),TLPE,ROEL,ROEL2,NEW
      COMMON/COM8/ROEA,ROEB,ROEC,ROEC2,CP0,CP1,CP2,CP3,
     1CF0,CF1,CF2,CGD1,CGD2,CGB1,CGB2,CGF1,CGF2
      IF (IQ-1) 100,101,102
  100 IP=2
      GO TO 200
  101 IP=1
      GO TO 200
  102 I=1
      IP=2
  105 DO 595 J=IP,LL
      IF(LCUT(J)) 595,510,595
  510 DRX=RX(J)-RX(I)
      IF(DRX) 513,517,517
  513 IF(DRX+ROE) 595,595,520
  517 IF(DRX-ROE) 520,595,595
  520 DRY=RY(J)-RY(I)
      IF(DRY) 523,527,527
  523 IF(DRY+ROE) 595,595,530
  527 IF(DRY-ROE) 530,595,595
  530 DRZ=RZ(J)-RZ(I)
      IF(DRZ) 533,537,537
  533 IF(DRZ+ROE) 595,595,540
  537 IF(DRZ-ROE) 540,595,595
  540 DIST=DRX*DRX+DRY*DRY+DRZ*DRZ
      IF(DIST-ROE2) 550,595,595
  550 DIST=SQRT(DIST)
  560 POT=EXP(PEXA+PEXB*DIST)-PPTC
  580 TPOT=TPOT+POT
      PPE(I)=PPE(I)+BSAVE*POT
      PPE(J)=PPE(J)+TSAVE*POT
  595 CONTINUE
  600 CONTINUE
C
  200 DO 300 I=IP,LD
```

```
      IF(LCUT(I)) 300,205,300
  205 IP=I+1
      DO 295 J=IP,LL
      IF(LCUT(J)) 295,210,295
  210 DRX=RX(J)-RX(I)
      IF(DRX) 213,217,217
  213 IF(DRX+ROEC) 295,295,220
  217 IF(DRX-ROEC) 220,295,295
  220 DRY=RY(J)-RY(I)
      IF(DRY) 223,227,227
  223 IF(DRY+ROEC) 295,295,230
  227 IF(DRY-ROEC) 230,295,295
  230 DRZ=RZ(J)-RZ(I)
      IF(DRZ) 233,237,237
  233 IF(DRZ+ROEC) 295,295,240
  237 IF(DRZ-ROEC) 240,295,295
  240 DIST=DRX*DRX+DRY*DRY+DRZ*DRZ
      IF(DIST-ROEC2) 250,295,295
  250 DIST=SQRT(DIST)
      IF(DIST-ROEA) 260,255,255
  255 IF(DIST-ROEB) 265,270,270
  260 POT=EXP(EXA+EXB*DIST)
      GO TO 280
  265 POT=DIST*(DIST*(DIST*CP3+CP2)+CP1)+CP0
      GO TO 280
  270 POT=EXP(CGD1+CGB1*DIST)-EXP(CGD2+CGB2*DIST)
  280 TPOT=TPOT+POT
      SAVE=0.5*POT
      PPE(I)=PPE(I)+SAVE
      PPE(J)=PPE(J)+SAVE
  295 CONTINUE
  300 CONTINUE
      RETURN
      END


C
C     SUBROUTINE PRINT PRINTS PERTINENT GENERAL DATA FOR
C     EACH TIMESTEP PRINTOUT.
C


C


      SUBROUTINE PRINT
C
C
      COMMON/COM1/RX(500),RY(500),RZ(500),LCUT(500),
     1LL,LD,ITYPE,NVAC
      COMMON/COM2/IH1(20),IH2(8),IHS(10),IHB(6),IHT(6),
     1TARGET(4),TMAS,BULLET(4),BMAS,PLANE,TEMP,THERM,DDTII,
     1DDTIF
      COMMON/COM3/RXI(500),RYI(500),RZI(500),CVR,EVR,
     1NT,TIME,DT,DTI,ILAY,RXK(500),RYK(500),RZK(500)
      COMMON/COM4/IX,IY,IZ,SCX,SCY,SCZ,IDEEP,D1X,D1Y,
     1D1Z,IVACX,IVACY,IVACZ
      COMMON/COM5/ROE,ROE2,ROEM,EXA,EXB,PEXA,PEXB,FXA,PFXA,
     1IQ,TSAVE,BSAVE
      COMMON/COM8/ROEA,ROEB,ROEC,ROEC2,CP0,CP1,CP2,CP3,
     1CF0,CF1,CF2,CGD1,CGD2,CGB1,CGB2,CGF1,CGF2
 9710 FORMAT(40X,10A4,/,28X,20A4,/)
 9720 FORMAT(9H TARGET -,4A4,10HPRIMARY - ,4A4,1X,14HLATTICE
     1 UNIT =,F7.4,4H ANG)
 9730 FORMAT(4X,6HMASS =,F7.2,13X,6HMASS =,F7.2,9X,14HLATTIC
     1E TEMP =F5.2,7H DEG K,,18H  THERMAL CUTOFF =,F5.2,3H E
     1V/)
 9740 FORMAT(2H (,A4,8H) PLANE,,18H  PRIMARY ENERGY =,
     1 F5.2,21HKEV,  CRYSTAL SIZE ( ,I2,3H X ,I2,3H X ,I2,3H
     1 ),, 4X, 16HVACANCY IN SITE , I4/)
 9741 FORMAT(2H (,A4,8H) PLANE,,18H  PRIMARY ENERGY =,
     1 F5.3,21HKEV,  CRYSTAL SIZE ( ,I2,3H X ,I2,3H X ,I2,
```

```
     13H ),, 4X,I3,' LAYERS ARE FREE TO MOVE',/)
 9742 FORMAT(2H (,A4,8H) PLANE,,18H  PRIMARY ENERGY =,
     1 F5.2,21HKEV,  CRYSTAL SIZE ( ,I2,3H X ,I2,3H X ,I2,3H
     1 ),, 4X, 20HREPLACEMENT IN SITE , I4/)
 9750 FORMAT(' IMPLANTATION AT SITE # ',I3,3X,'X=',I2,4X,
     1'Y=',I2,4X,'Z=',I2,5X,'IQ=',I2,4X,'DDTII=',F6.4,4X,
     1'DDTIF=',F6.4,//,' LATTICE ATOM START POINT',5X,
     1'X=',F5.2,3X,'Y=',F5.2,3X,'Z=',F5.2,6X,'INTERSTITIAL
     1START POINT',5X,'X=',F5.2,3X,'Y=',F5.2,3X,'Z=',
     1F5.2,,//)
 9760 FORMAT(12H POTENTIAL  ,6A4,3X,5HPEXA=,F9.5,2X,5HPEXB=,
     1F9.5,2X,5HPFXA=,F9.5)
 9765 FORMAT(12X,6A4,3X,5HEXA =,F9.5,2X,5HEXB =,F9.5,2X,5HFX
     1A =,F9.5/)
 9770 FORMAT(' WHEN',F8.4,' < R <',F8.4,' THE MATCHING POTEN
     1TIAL PARAMETERS ARE',//,'        CP0 =',F10.3,', CP1 ='
     1F10.3,', CP2 =',F10.3,', CP3 =',F10.3,/,'        CF0 ='
     1E10.3,', CF1 =',E10.3,', CF2 =',E10.3,//)
 9780 FORMAT(' CUT-OFF AT',F5.2,', WHEN R > ',F6.3,' LU, MOR
     1SE POTENTIAL PARAMETERS ARE', 8A4,//,10X,'   CGD1 =',
     1F8.4,', CGD2 =',F8.4,', CGB1 =',F8.4,', CGB2 =',F8.4,
     1', CGF1 =',F8.4,', CGF2 =',F8.4,//)
 9791 FORMAT(36X,'DDTII=',F6.4/,36X,'DDTIF=',F6.4)
       WRITE ( 6,9710) IHS,IH1
       WRITE ( 6,9720) TARGET,BULLET,CVR
       WRITE ( 6,9730) TMAS,BMAS,TEMP,THERM
      GO TO (401,402,403,402), ITYPE
  401  WRITE ( 6,9740) PLANE,EVR,IX,IY,IZ,NVAC
      GO TO 405
  402 WRITE (6,9741) PLANE,EVR,IX,IY,IZ,ILAY
      GO TO 405
  403  WRITE ( 6,9742) PLANE,EVR,IX,IY,IZ,NVAC
       WRITE ( 6,9760) IHB,PEXA,PEXB,PFXA
       WRITE ( 6,9765) IHT,EXA,EXB,FXA
       WRITE ( 6,9770) ROEA,ROEB,CP0,CP1,CP2,CP3,CF0,CF1,CF2
       WRITE ( 6,9780) ROEC,ROEB,IH2,CGD1,CGD2,CGB1,CGB2,
     1CGF1,CGF2
       WRITE ( 6,9790) NT,DTI,TIME,DT
      RETURN
      END
C

****************************************************************

                ***********************************
C                     'PLUCK CONFIGURATION'
                ***********************************


C
C      SUBROUTINE PLUCK CHOOSES THE ATOMS WHICH WILL
C     MAKE UP THE SMALLER CRYSTAL USED IN INITIAL DYNAMIC
C     CALCULATIONS. PERTINENT DATA FOR THIS SMALLER
C     CRYSTAL AND POSITIONS OF ALL ATOMS OF THIS CRYSTAL
C     CAN THEN BE PUNCHED  OUT ON DATA CARDS TO BE USED AS
C     INPUT TO THE DYNAMIC PROGRAM.
C



      SUBROUTINE PLUCK
      COMMON/COM1/RX(500),RY(500),RZ(500),LCUT(500),
     1LL,LD,ITYPE,NVAC
      COMMON/COM4/IX,IY,IZ,SCX,SCY,SCZ,IDEEP,D1X,D1Y,D1Z,
     1IVACX,IVACY,IVACZ
      COMMON/COM10/IXNEW,IYNEW,IZNEW,II
      COMMON/COM11/RXNEWI(250),RYNEWI(250),RZNEWI(250),
     1KEEP(250),NNUM(250)
 1500 IXNEW=7
      IYNEW=IVACY+3
```

```
      IZNEW=7
      NM=5
      NI=8
      II=2
      MM=0
      NX=16
      NII3=10
      NII4=5
      IF(IYNEW.EQ.3) GO TO 1514
      IF(IYNEW.EQ.5) GO TO 1514
 1505 DO 1509 I=II,NM
      NNUM(I)=NI
 1509 NI=NI+1
      NI=NI+1
      II=II+4
      NM=NM+4
      IF (II.LE.NX) GO TO 1505
      NX=NX+9
      NI=NI+NII4
      MM=MM+1
      IF(IYNEW.EQ.MM) GO TO 1600
      NM=NM-1
      GO TO 1515
 1514 NX=9
      NM=4
      NII3=4
      NII4=11
 1515 DO 1520 I=II,NM
      NNUM(I)=NI
 1520 NI=NI+1
      NI=NI+2
      II=II+3
      NM=NM+3
      IF(II.LE.NX) GO TO 1515
      NX=NX+16
      NI=NI+NII3
      MM=MM+1
      IF(IYNEW.EQ.MM) GO TO 1600
      NM=NM+1
      GO TO 1505
 1600 II=II-1
      RXNEWI(1)=RX(1)
      RYNEWI(1)=RY(1)
      RZNEWI(1)=RZ(1)
      KEEP(1)=1
      NNUM(1)=1
 1700 DO 1750 I=2,II
      RXNEWI(I)=RX(NNUM(I))
      RYNEWI(I)=RY(NNUM(I))
      RZNEWI(I)=RZ(NNUM(I))
      KEEP(I)=NNUM(I)
 1750 CONTINUE
      RETURN
      END
************************************************************


      BLOCK DATA
      COMMON/COM1/RX(1000),RY(1000),RZ(1000),LCUT(1000),
     1LL,LD,ITYPE,NVAC
      DATA RX/1000*0.0/,RY/1000*0.0/,RZ/1000*0.0/,
     1LCUT/1000*0.0/
      COMMON/COM3/RXI(1000),RYI(1000),RZI(1000),CVR,EVR,
     1NT,TIME,DT,DTI,ILAY,RXK(1000),RYK(1000),RZK(1000)
      DATA RXI/1000*0.0/,RYI/1000*0.0/,RZI/1000*0.0/
      COMMON/COM6/FX(1000),FY(1000),FZ(1000),PAC,PFPTC,FM
      DATA FX/1000*0.0/,FY/1000*0.0/,FZ/1000*0.0/
      END
```

COMPUTER PROGRAM
FOR DYNAMIC SIMULATIONS

THE DYNAMIC PROGRAM IS USED TO DETERMINE THE MINIMUM ENERGY REQUIRED IN A SPECIFIC DIRECTION TO CAUSE AN INTERSTITIAL ATOM TO EXIT FROM THE CRYSTAL. THE COMPUTATIONS REQUIRED ARE ESSENTIALLY THE SAME AS THOSE IN THE STATIC SIMULATIONS. CONSEQUENTLY,COMMENTS WILL ONLY BE INCLUDED TO POINT OUT SIGNIFICANT DIFFERENCES FROM THE STATIC PROGRAM. TWO CONFIGURATIONS OF THE DYNAMIC PROGRAM EXIST:

(1) THE ENTIRE CRYSTAL CONFIGURATION - THE ENTIRE 250 ATOM CRYSTAL IS USED IN ALL CALCULATIONS.

(2) THE PLUCK CONFIGURATION - A SMALLER CRYSTAL DETERMINED BY SUBROUTINE PLUCK IS USED FOR ALL CALCULATIONS.

```
      DIMENSION VX(1000),VY(1000),VZ(1000),PKE(1000)
      DIMENSION DX(1000),DY(1000),DZ(1000),PTE(1000)
      DIMENSION RXK(1000),RYK(1000),RZK(1000)
      DIMENSION KEEP(500)
      COMMON/COM1/RX(1000),RY(1000),RZ(1000),LCUT(1000),
     1LL,LD,ITYPE,NVAC
      COMMON/COM2/IH1(20),IH2(8),IHS(10),IHB(6),IHT(6),
     1TARGET(4),TMAS,BULLET(4),BMAS,PLANE,TEMP,THERM
      COMMON/COM3/RXI(1000),RYI(1000),RZI(1000),CVR,EVR,
     1NT,TIME,DT,DTI,ILAY
      COMMON/COM4/IX,IY,IZ,SCX,SCY,SCZ,IDEEP,D1X,D1Y,D1Z
      COMMON/COM5/ROE,ROE2,ROEM,EXA,EXB,PEXA,PEXB,FXA,PFXA,
     1IQ,TSAVE,BSAVE,CX,CY,CZ
      COMMON/COM6/FX(1000),FY(1000),FZ(1000),PAC,PFPTC,FM
      COMMON/COM7/PPTC,TPOT,PPE(1000),TLPE,ROEL,ROEL2,NEW
      COMMON/COM8/ROEA,ROEB,ROEC,ROEC2,CP0,CP1,CP2,CP3,
     1CF0,CF1,CF2,CGD1,CGD2,CGB1,CGB2,CGF1,CGF2
      COMMON/COM9/RXSAVE,RYSAVE,RZSAVE
      COMMON/COMA/ A(4,5),MCRO
C
 9010 FORMAT(20A4)
 9020 FORMAT(8A4,3F8.5,2F5.2)
 9030 FORMAT(4A4,3F8.5,6A4,F6.2)
 9040 FORMAT(F6.5,5X,I5,6I4,3F5.2)
 9050 FORMAT(10A4,A4,4I3,F8.4,I4,F5.3)
C
 9610 FORMAT(1H1)
 9620 FORMAT(47X,'SUMMARY OF ATOMS'//,35X,8A4,', NT ='I4,//,
     13(' ATOM          POSITION            BIND ENERGY     '),//)
 9630 FORMAT(3(I5,3F6.2,F8.4,8X))
 9640 FORMAT(/4X,F10.3,25H EV,TOTAL KINETIC ENERGY,,F10.3,
     127H EV,TOTAL POTENTIAL ENERGY,F10.3,' EV, REDUCTION',/
     1/60X,'RADIUS =',F5.2,)
 9650 FORMAT(105X,4HPAGE,I3,/,1H1)
 9660 FORMAT(/  '      ATOM      DX          DY          DZ
     1VX          VY          VZ          KE          PE          TE',/)
 9670 FORMAT(1I8,3F10.3,3F10.1,3F10.4 )
 9680 FORMAT(' SHARP DT DECREASE',2E10.3)


*******************************************************

                    **************************************
C                     'ENTIRE CRYSTAL CONFIGURATION'
                    **************************************


 9690 FORMAT(I4,3F5.2,I4)
 9691 FORMAT(9F8.4)
```

```
                ***********************************
C                        'PLUCK CONFIGURATION'
                ***********************************

 9690 FORMAT(I4,3F5.2,4(I4))
 9691 FORMAT(I5,3(1X,F8.4),1X,I5)

************************************************************

C
      RUNTM=4*60-20
      START=0.01*ITIME(XX)
      DO 2 I=1,1000
      RXK(I)=0.0
      RYK(I)=0.0
      RZK(I)=0.0
      VX(I)=0.0
      VY(I)=0.0
      VZ(I)=0.0
      PKE(I)=0.0
      PPE(I)=0.0
      PTE(I)=0.0
    2 RZI(I)=0.0
      ISHUT=1
      NRUN=0
C
       READ ( 5,9010) IH1
       READ ( 5,9020) IH2,DCON,ALPHA,RE,ROEC,ROEL
       READ ( 5,9030) BULLET,BMAS,PEXA,PEXB,IHB,THERM
       READ ( 5,9030) TARGET,TMAS,EXA,EXB,IHT,TEMP
C
      ROE2=3.0
       READ ( 5,9050) IHS,PLANE,LS,IX,IY,IZ,CVR,MCRO ,DTI
      ROE=SQRT(ROE2)
      ROEM = ROE-DTI
      ROEL2=ROEL*ROEL
      CVE=1.60E-19
      CVM=1.672E-27
      FM=1.0E-10
      FM2=FM*FM
      CVD=CVR*1.0E-10
      CVED=CVE/CVD
      PTMAS=TMAS*CVM
      PBMAS=BMAS*CVM
      HTMAS=0.5*PTMAS/CVE
      HBMAS=0.5*PBMAS/CVE
      VFAC=1.0
      TSAVE=BMAS/(BMAS+TMAS)
      BSAVE=TMAS/(BMAS+TMAS)
C
      FXA=ALOG(-EXB*CVED)+EXA
      PFXA=ALOG(-PEXB*CVED)+PEXA
      PPTC=EXP(PEXA+PEXB*ROE)
      PAC=ALOG(CVED)+PEXA
      PFPTC=EXP(PAC+PEXB*ROE)
C
      CGD1=ALOG(DCON)+2.0*ALPHA*RE
      CGD2=ALOG(2.0*DCON)+ALPHA*RE
      CGB1=-2.0*ALPHA*CVR
      CGB2=-ALPHA*CVR
      CGF1=ALOG(-CGB1*CVED)+CGD1
      CGF2=ALOG(-CGB2*CVED)+CGD2
C
      ROEA=1.50/CVR
      ROEB=2.0/CVR
      ROEC2=ROEC*ROEC
C
      A(1,1)=1.0
      A(1,2)=ROEA
```

```
      A(1,3)=ROEA*ROEA
      A(1,4)=ROEA**3
      A(1,5)=EXP(EXA+EXB*ROEA)
      A(2,1)=1.0
      A(2,2)=ROEB
      A(2,3)=ROEB*ROEB
      A(2,4)=ROEB**3
      A(2,5)=EXP(CGD1+CGB1*ROEB)-EXP(CGD2+CGB2*ROEB)
      A(3,1)=0.0
      A(3,2)=-1.0
      A(3,3)=-2.0*ROEA
      A(3,4)=-3.0*ROEA*ROEA
      A(3,5)=EXP(EXA+EXB*ROEA)/CVED
      A(4,1)=0.0
      A(4,2)=-1.0
      A(4,3)=-2.0*ROEB
      A(4,4)=-3.0*ROEB*ROEB
      A(4,5)=(EXP(CGF1+CGB1*ROEB)-EXP(CGF2+CGB2*ROEB))/CVED
      CALL CROSYM
      CP0=A(1,5)
      CP1=A(2,5)
      CP2=A(3,5)
      CP3=A(4,5)
      CF0=-CP1*CVED
      CF1=-2.0*CP2*CVED
      CF2=-3.0*CP3*CVED
    5  READ ( 5,9040) EVR,NTT,NS,ND,IP,IDEEP,ITYPE,NVAC,D1X,
     1D1Y,D1Z
      IF(NTT.EQ.0) GO TO 9999
      IQ=ITYPE-1
      NTTS=NTT
      EV=EVR*1.0E+3

*******************************************************************

                    *********************************
C                           'PLUCK CONFIGURATION'
                    *********************************


C
C     DATA FOR THE PLUCK CRYSTAL IS READ INTO THE COMPUTER
C     AND APPROPRIATE PARAMETERS ARE CORRELATED. THIS
C     CREATES THE CRYSTAL TO BE USED IN THE SIMULATION.
C


      READ  (5,9690) LL,D1X,D1Y,D1Z,NVAC,IXNEW,IYNEW,IZNEW
      II=60
      LL=II
      IX=IXNEW
      IY=IYNEW
      IZ=IZNEW
      DO 15  I=1,LL
      READ  (5,9691)  I,RX(I),RY(I),RZ(I),KEEP(I)
   15 CONTINUE


                    *********************************
C                     'ENTIRE CRYSTAL CONFIGURATION'
                    *********************************


C
C     DATA FOR THE ENTIRE CRYSTAL IS READ INTO THE COMPUTER.
C     THIS CREATES THE CRYSTAL TO BE USED IN THE SIMULATION.
C


       READ  (5,9690) LL,D1X,D1Y,D1Z,NVAC
```

```
      DO 15 I=1,LL,3
      K=I+1
      J=I+2
       READ  (5,9691) RX(I),RY(I),RZ(I),RX(K),RY(K),RZ(K),
     1RX(J),RY(J),RZ(J)


*********************************************************************
   30 ILAY=IDEEP
      IF(IDEEP) 35,35,40
   35 LD=LL
      ILAY=IY
   40 DO 45 I=1,LL
      RXK(I)=RX(I)
      RYK(I)=RY(I)
      RZK(I)=RZ(I)
      RXI(I)=RX(I)
      RYI(I)=RY(I)
   45 RZI(I)=RZ(I)
      RXI(1)=RX(1)
      RYI(1)=RY(1)
      RZI(1)=RZ(1)
      RXK(1)=RX(1)
      RYK(1)=RY(1)
      RZK(1)=RZ(1)
C
      TPOT=0.0
      CALL ENERGY
      BIND=-TPOT
      TE=TPOT+BIND
      TPKE=EV
      TE=TPOT+BIND+TPKE
       WRITE ( 6,9610)
       WRITE ( 6,9620) IH2,NT
      DO 70 I=1,LL,3
      K=I+1
      J=I+2
   70  WRITE (6,9630) KEEP(I),RX(I),RY(I),RZ(I),PPE(I),
     1KEEP(K),RX(K),RY(K),RZ(K),PPE(K),KEEP(J),RX(J),RY(J),
     1RZ(J),PPE(J)
       WRITE ( 6,9640) TPKE,TPOT,TE,ROEL
      NPAGE=1
       WRITE ( 6,9650) NPAGE


C
C     APPROPRIATE IMPACT POINTS FOR INTERSTITIAL ESCAPE ARE
C     CHOSEN AND AN IMPACT POINT GENERATOR IS CREATED TO
C     GENERATE AND THEN TEST POSSIBLE DIRECTIONS OF ESCAPE.
C


      CX=3.8
      CY=0.00
      CZ=3.6
      NTT=NTTS
      DO 3000 II=1,4
      CX=CX+0.4
      DO 3000  JJ=1,3
      CZ=CZ+0.4
      RXSAVE=CX
      RYSAVE=CY
      RZSAVE=CZ
      AC=SQRT((CX-RXI(1))**2+(CY-RYI(1))**2+(CZ-RZI(1))**2)
      COX=(CX-RXI(1))/AC
      COY=(CY-RYI(1))/AC
      VOL=SQRT(EV/HBMAS)
      VX(1)=VOL*COX
      VY(1)=VOL*COY
      COZ=(CZ-RZI(1))/AC
      VZ(1)=VOL*COZ
      IF(NRUN.EQ.0) GO TO 60
```

```
   50 DO 55 I=1,LL
      LCUT(I)=0
      RX(I)=RXI(I)
      RY(I)=RYI(I)
      RZ(I)=RZI(I)
      RXK(I)=RXI(I)
      RYK(I)=RYI(I)
   55 RZK(I)=RZI(I)
   60 NRUN=1
      DO 65 I=2,LL
      VX(I)=0.0
      VY(I)=0.0
      VZ(I)=0.0
      PPE(I)=0.0
      PKE(I)=0.0
   65 PTE(I)=0.0
      TPOT=0.0
      NEW=0
C
      TIME=0.0
      NT=0
      IF (NRUN.GT.1.0) GO TO 95
      NPAGE=NPAGE+1
C
   95 TFAC=2.0*PTMAS*DTI*CVD
      TFACB=2.0*PBMAS*DTI*CVD
      DT=1.0E-17
  100 DTOD=DT/CVD
      HDTOD=0.5*DTOD
      DTOM=DT/PTMAS
      HDTOM=0.5*DTOM
      DTOMB=DT/PBMAS
      HDTOMB=0.5*DTOMB
  200 CALL STEP
      IF(LCUT(1).GT.0) GO TO 240
      I=1
      RXK(I)=RX(I)
      RYK(I)=RY(I)
      RZK(I)=RZ(I)
      RX(I)=RX(I)+DTOD*(HDTOMB*FX(I)+VX(I))
      RY(I)=RY(I)+DTOD*(HDTOMB*FY(I)+VY(I))
      RZ(I)=RZ(I)+DTOD*(HDTOMB*FZ(I)+VZ(I))
  240 DO 245 I=2,LD
      IF(LCUT(I).GT.0)GO TO 245
      RXK(I)=RX(I)
      RYK(I)=RY(I)
      RZK(I)=RZ(I)
      RX(I)=RX(I)+DTOD*(HDTOM*FX(I)+VX(I))
      RY(I)=RY(I)+DTOD*(HDTOM*FY(I)+VY(I))
      RZ(I)=RZ(I)+DTOD*(HDTOM*FZ(I)+VZ(I))
  245 CONTINUE
      CALL STEP
      EMAX=0.0
      FMAX=0.0
      TIME=TIME+DT
      NT=NT+1
      IF(LCUT(1).GT.0) GO TO 265
      I=1
      VSS=VX(I)
      VX(I)=VSS+HDTOMB*FX(I)
      RX(I)=RXK(I)+(VX(I)+VSS)*HDTOD
      VSS=VY(I)
      VY(I)=VSS+HDTOMB*FY(I)
      RY(I)=RYK(I)+(VY(I)+VSS)*HDTOD
      VSS=VZ(I)
      VZ(I)=VSS+HDTOMB*FZ(I)
      RZ(I)=RZK(I)+(VZ(I)+VSS)*HDTOD
      PKE(I)=VX(I)*VX(I)+VY(I)*VY(I)+VZ(I)*VZ(I)
      EMAX=PKE(I)
  260 FX(I)=0.0
      FY(I)=0.0
      FZ(I)=0.0
```

```
  265 DO 280 I=2,LD
      IF(LCUT(I).GT.0)GO TO 280
      VSS=VX(I)
      VX(I)=VSS+HDTOM*FX(I)
      RX(I)=RXK(I)+(VX(I)+VSS)*HDTOD
      VSS=VY(I)
      VY(I)=VSS+HDTOM*FY(I)
      RY(I)=RYK(I)+(VY(I)+VSS)*HDTOD
      VSS=VZ(I)
      VZ(I)=VSS+HDTOM*FZ(I)
      RZ(I)=RZK(I)+(VZ(I)+VSS)*HDTOD
      PKE(I)=VX(I)*VX(I)+VY(I)*VY(I)+VZ(I)*VZ(I)
      FX(I)=0.0
      FY(I)=0.0
      FZ(I)=0.0
      IF(PKE(I).GT.EMAX) EMAX=PKE(I)
  280 CONTINUE
      DTL=DT
      IF(EMAX.EQ.0.0) GO TO 285
      GO TO 290
  285 DT=1.0E-17
      GO TO 300
  290 DT=DTI*CVD/SQRT(EMAX)
      CTIME=0.01*ITIME(XX)-START
  300 IF(ISHUT.EQ.-1) GO TO 400
  310 IF(NS-NT) 400,400,100
  400 CALL PRINT
C
  410 TPOT=0.0
      DO 450 I=1,LL
      PPE(I)=0.0
  450 PTE(I)=0.0
      CALL ENERGY
      PKE(1)=HBMAS*PKE(1)
      TPKE=PKE(1)
      PTE(1)=PKE(1)+PPE(1)
      DO 620 I=2,LL
      PKE(I)=HTMAS*PKE(I)
      TPKE=TPKE+PKE(I)
  620 PTE(I)=PKE(I)+PPE(I)
      TE=TPOT+BIND
       WRITE ( 6,9660)
      DTEST=(RY(1)-RYI(1))**2
      IF (DTEST.GT. 0.01) DTEST= 0.01
  700 DO 750 I=1,LD
      DX(I)=RX(I)-RXI(I)
      DY(I)=RY(I)-RYI(I)
      DZ(I)=RZ(I)-RZI(I)
      IF (DX(I)**2.GE.DTEST) GO TO 720
      IF (DY(I)**2.GE.DTEST) GO TO 720
      IF (DZ(I)**2.GE.DTEST) GO TO 720
      IF(PPE(I).GE.-3.0) GO TO 720
      GO TO 750
C

************************************************************

                 ***********************************
C                       'PLUCK CONFIGURATION'
                 ***********************************


C
C     IN ORDER TO FOLLOW THE LOGIC OF THE DYNAMIC PROGRAM
C     THE ATOMS CREATED BY SUBROUTINE PLUCK HAVE BEEN
C     RENUMBERED CONSECUTIVELY FROM ATOM NUMBER 1, BUT THE
C     ATOM NUMBER OF EACH ATOM AS IT WAS IN THE ORIGINAL
C     CRYSTAL HAS BEEN SAVED IN AN ARRAY. THE WRITE COMMANDS
C     MUST THEREFORE PRINT THE ARRAY KEEP(I) SO THAT
C     PRINTED OUTPUT WILL BE IN A FORM TO ALLOW READY
C     COMPARISON WITH THE ORIGINAL CRYSTAL. TO ACCOMPLISH
```

```
C     THIS IN THE PLUCK CONFIGURATION, THE STATEMENTS NUM-
C     BERED 720 AND 965 SHOULD BE CHANGED TO READ:
C


  720  WRITE(6,9670) KEEP(I),DX(I),DY(I),DZ(I),VX(I),VY(I),
     1VZ(I),PKE(I),PPE(I),PTE(I)

  965  WRITE (6,9630) KEEP(I),RX(I),RY(I),RZ(I),PPE(I),
     1KEEP(K),RX(K),RY(K),RZ(K),PPE(K),KEEP(J),RX(J),RY(J),
     1RZ(J),PPE(J)

*************************************************************


  720  WRITE ( 6,9670) I,DX(I),DY(I),DZ(I),VX(I),VY(I),
     1VZ(I),PKE(I),PPE(I),PTE(I)
  750 CONTINUE
       WRITE ( 6,9640) TPKE,TPOT,TE,ROEL
       WRITE ( 6,9650) NPAGE
      NPAGE=NPAGE+1
      IF(NT-NTT) 790,950,950
  790 NS=NS+ND
      GO TO 100
  950 CONTINUE
      NS=0
C
  955  WRITE ( 6,9620) IH2,NT
      DO 965 I=1,LL,3
      K=I+1
      J=I+2
  965  WRITE ( 6,9630) I,RX(I),RY(I),RZ(I),PPE(I),K,RX(K),
     1RY(K),RZ(K),PPE(K),J,RX(J),RY(J),RZ(J),PPE(J)
       WRITE ( 6,9640) TPKE,TPOT,TE,ROEL
       WRITE ( 6,9650) NPAGE


C
C     AFTER CALCULATIONS OF THE DYNAMICS ASSOCIATED WITH
C     ALL IMPACT POINTS ALONG A (100) DIRECTION, THE IMPACT
C     POINT GENERATOR MUST BE INCREMENTED.
C


      IF(JJ.EQ.3) CZ=3.6
 1000 IF(ISHUT) 9999,3000,3000
 3000 CONTINUE
 9999 STOP
      END
C


C
C     SUBROUTINES B100, PLACE, AND PLUCK ARE NOT USED IN
C     DYNAMIC SIMULATIONS. SUBROUTINES STEP, CROYSM, AND
C     ENERGY ARE USED IN THE SAME FORM AS IN THE STATIC
C     SIMULATIONS AND ARE NOT REPEATED HERE.  SUBROUTINE
C     PRINT APPEARS IN DYNAMIC SIMULATIONS AS FOLLOWS:
C



      SUBROUTINE PRINT
C
C
      COMMON/COM1/RX(1000),RY(1000),RZ(1000),LCUT(1000),
     1LL,LD,ITYPE,NVAC
      COMMON/COM2/IH1(20),IH2(8),IHS(10),IHB(6),IHT(6),
     1TARGET(4),TMAS,BULLET(4),BMAS,PLANE,TEMP,THERM
      COMMON/COM3/RXI(1000),RYI(1000),RZI(1000),CVR,EVR,
     1NT,TIME,DT,DTI,ILAY
```

```
      COMMON/COM4/IX,IY,IZ,SCX,SCY,SCZ,IDEEP,D1X,D1Y,D1Z
      COMMON/COM5/ROE,ROE2,ROEM,EXA,EXB,PEXA,PEXB,FXA,PFXA,
     1IQ,TSAVE,BSAVE,CX,CY,CZ
      COMMON/COM8/ROEA,ROEB,ROEC,ROEC2,CP0,CP1,CP2,CP3,
     1CF0,CF1,CF2,CGD1,CGD2,CGB1,CGB2,CGF1,CGF2
      COMMON/COM9/RXSAVE,RYSAVE,RZSAVE
 9710 FORMAT(40X,10A4,/,28X,20A4,/)
 9720 FORMAT(9H TARGET -,4A4,10HPRIMARY - ,4A4,1X,14HLATTICE
     1 UNIT =,F7.4,4H ANG)
 9730 FORMAT(4X,6HMASS =,F7.2,13X,6HMASS =,F7.2,9X,14HLATTIC
     1E TEMP =F5.2,7H DEG K,,18H  THERMAL CUTOFF =,F5.2,3H E
     1V/)
 9740 FORMAT(2H (,A4,8H) PLANE,,18H  PRIMARY ENERGY =,
     1 F5.2,21HKEV,  CRYSTAL SIZE ( ,I2,3H X ,I2,3H X ,I2,3H
     1 ),, 4X, 16HVACANCY IN SITE , I4/)
 9741 FORMAT(2H (,A4,8H) PLANE,,18H  PRIMARY ENERGY =,
     1 F6.5,21HKEV,  CRYSTAL SIZE ( ,I2,3H X ,I2,3H X ,I2,
     13H ),, 4X, 16HINTERSTITIAL (-,F5.2,2H,-,F5.2,2H,+,
     1F5.2,12H) FROM SITE ,I4/)
 9742 FORMAT(2H (,A4,8H) PLANE,,18H  PRIMARY ENERGY =,
     1 F5.2,21HKEV,  CRYSTAL SIZE ( ,I2,3H X ,I2,3H X ,I2,3H
     1 ),, 4X, 20HREPLACEMENT IN SITE , I4/)
 9750 FORMAT (' PRIMARY START POINT (LU)  X=',F5.2,',  Y=',
     1F5.2,',  Z=',F5.2,5X,I3,' LAYERS ARE FREE TO MOVE',
     110X,'IQ=',I2)
 9751 FORMAT (' OFFSET FROM EQUILIB (LU) OX=',F5.2,',OY=',
     1F5.2,',OZ=',F5.2,5X,'PRIMARY ENERGY IS',F6.3,' KEV',/)
 9760 FORMAT(12H POTENTIAL  ,6A4,3X,5HPEXA=,F9.5,2X,5HPEXB=,
     1F9.5,2X,5HPFXA=,F9.5)
 9765 FORMAT(12X,6A4,3X,5HEXA =,F9.5,2X,5HEXB =,F9.5,2X,5HFX
     1A =,F9.5/)
 9770 FORMAT(' WHEN',F8.4,' < R <',F8.4,' THE MATCHING POTEN
     1TIAL PARAMETERS ARE',//,'        CP0 =',F10.3,', CP1 ='
     1F10.3,', CP2 =',F10.3,', CP3 =',F10.3,/,'        CF0 ='
     1E10.3,', CF1 =',E10.3,', CF2 =',E10.3,//)
 9780 FORMAT(' CUT-OFF AT',F5.2,', WHEN R > ',F6.3,' LU, MOR
     1SE POTENTIAL PARAMETERS ARE', 8A4,//,10X,'   CGD1 =',
     1F8.4,', CGD2 =',F8.4,', CGB1 =',F8.4,', CGB2 =',F8.4,
     1', CGF1 =',F8.4,', CGF2 =',F8.4,//)
  9790 FORMAT(10H TIMESTEP ,I4,22X,6HDTI = , F5.4, 5H LU,
     1,22H  ELAPSED TIME (SEC) =, E10.4,', NEXT TIMESTEP IS
     1=',E10.4/)
        WRITE ( 6,9710) IHS,IH1
        WRITE ( 6,9720) TARGET,BULLET,CVR
        WRITE ( 6,9730) TMAS,BMAS,TEMP,THERM
      GO TO (401,402,403,402), ITYPE
  401   WRITE ( 6,9740) PLANE,EVR,IX,IY,IZ,NVAC
      GO TO 405
  402   WRITE ( 6,9741) PLANE,EVR,IX,IY,IZ,D1X,D1Y,D1Z,NVAC
      GO TO 405
  403   WRITE ( 6,9742) PLANE,EVR,IX,IY,IZ,NVAC
  405   WRITE ( 6,9750) RXI(1),RYI(1),RZI(1),ILAY,IQ
      WRITE(6,9751) RXSAVE,RYSAVE,RZSAVE,EVR
        WRITE ( 6,9760) IHB,PEXA,PEXB,PFXA
        WRITE ( 6,9765) IHT,EXA,EXB,FXA
        WRITE ( 6,9770) ROEA,ROEB,CP0,CP1,CP2,CP3,CF0,CF1,CF2
        WRITE ( 6,9780) ROEC,ROEB,IH2,CGD1,CGD2,CGB1,CGB2,
     1CGF1,CGF2
        WRITE ( 6,9790) NT,DTI,TIME,DT
      RETURN
      END


      BLOCK DATA
      COMMON/COM1/RX(1000),RY(1000),RZ(1000),LCUT(1000),
     1LL,LD,ITYPE,NVAC
      DATA RX/1000*0.0/,RY/1000*0.0/,RZ/1000*0.0/,
     1LCUT/1000*0.0/
      COMMON/COM3/RXI(1000),RYI(1000),RZI(1000),CVR,EVR,
     1NT,TIME,DT,DTI,ILAY
      DATA RXI/1000*0.0/,RYI/1000*0.0/,RZI/1000*0.0/
      COMMON/COM6/FX(1000),FY(1000),FZ(1000),PAC,PFPTC,FM
```

```
DATA FX/1000*0.0/,FY/1000*0.0/,FZ/1000*0.0/
END
```

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DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY *(Corporate author)* Naval Postgraduate School Monterey, California 93940	2a. REPORT SECURITY CLASSIFICATION Unclassified
	2b. GROUP

3. REPORT TITLE

Computer Simulation of Inert Gas Interstitials in Tungsten

4. DESCRIPTIVE NOTES *(Type of report and, inclusive dates)*

Master's Thesis; December 1972

5. AUTHOR(S) *(First name, middle initial, last name)*

Richard D. Williams, III.

6. REPORT DATE December 1972	7a. TOTAL NO. OF PAGES 101	7b. NO. OF REFS 18
8a. CONTRACT OR GRANT NO.	9a. ORIGINATOR'S REPORT NUMBER(S)	
b. PROJECT NO.		
c.	9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)*	
d.		

10. DISTRIBUTION STATEMENT

Approved for public release; distribution unlimited.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY Naval Postgraduate School Monterey, California 93940

13. ABSTRACT

Computer simulation techniques were used to determine equilibrium positions and binding energies of inert gas atoms implanted in a tungsten crystal and to investigate the potential wells around these equilibrium positions in both perfect lattices and relaxed lattices. Stable positions were found for inert gas interstitials near lattice atoms in the third and fourth layers of the crystal. Interstitial positions near atoms in the first and second layers of the crystal appeared to be unstable if they exist at all. As a result of potential well studies, it was concluded that the mechanism associated with equilibrium position formation was a combination of local liquefaction of the lattice structure and interaction of the interstitial with lattice atoms. Equilibrium positions were found to be ill-defined regions in the general ⟨110⟩ direction. The binding energy determined for an interstitial site near a lattice atom in the third layer of the crystal was in excellent agreement with experimental results.

KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Implanted Atoms						
Interstitial Atoms						
Simulation						
Defect Binding Energy						

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Thesis
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c.2 Computer simulation of
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