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GRAINS--A QUASI-DYNAMIC CODE
FOR COMPUTER SIMULATION EXPERIMENTS
OF POINT AND LINE DEFECTS IN METALS

JANUARY 1970

AEC RESEARCH &
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UNITED STATES ATOMIC ENERGY COMMISSION UNDER CONTRACT AT(45-1)-1830

BNWL-1248
UC-32, Mathematics
and Computers

GRAINS--A QUASI-DYNAMIC CODE
FOR COMPUTER SIMULATION EXPERIMENTS
OF POINT AND LINE DEFECTS IN METALS*

R. E. Dahl, J. R. Beeler, Jr.**
and R. D. Bourquin

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January 1970

FIRST UNRESTRICTED
DISTRIBUTION JAN 28 '70

- * This report is based on work performed under United States Atomic Energy Commission Contracts AT(45-1)-1830 (R. E. Dahl, Jr. and R. D. Bourquin) and AT(40-1)-3912 (J. R. Beeler, Jr.)

A portion of this work is based on a research project submitted by Roy E. Dahl in partial fulfillment of the requirements for the degree of Doctorate of Philosophy at North Carolina State University, Department of Nuclear Engineering.

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BATTELLE MEMORIAL INSTITUTE
PACIFIC NORTHWEST LABORATORIES
RICHLAND, WASHINGTON 99352

Printed in the United States of America
Available from
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U.S. Department of Commerce
Springfield, Virginia 22151
Price: Printed Copy \$3.00; Microfiche \$0.65

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ABSTRACT

This report describes in detail the development of a computer code which is being used for computer simulation experiments on point and line defects in metals. The dynamic method of computer experimentation is used with an energy quench mode for accelerated convergence. It has been used in studies of grain boundaries and vacancy and interstitial complexes in iron and nickel. The results obtained for formation, migration and interfacial energies are in close agreement with those from other computer experiments and laboratory measurements.

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INTRODUCTION

The code GRAINS was developed for computer experimentation in simulation of point and line defects in metals on a UNIVAC-1108 computer. The computer experiment begins with a three dimensional array of atoms which are moved about, according to the forces exerted upon them by surrounding atoms, until an equilibrium configuration is attained. In this situation, the forces on all atoms are balanced, and the potential energy of the system is at its lowest possible value. Constraints on the system in the form of cell boundaries are imposed so that the inherent characteristics of the material, such as the lattice constant, elastic constants, and compressibility, can be maintained. The problems studies using this code include point and extended defects added to crystals. Equilibrium is attained when all atoms relax (i.e., move) to positions in which the forces upon them are balanced.

SUMMARY

GRAINS is a computer code which uses the dynamic method of solution. This method, which is described in depth by Beeler (1966), is based upon the movement of an assemblage of particles according to the classical equation of motion as dictated by a chosen interaction potential. The dynamic method was chosen because it is least likely to arrive at solutions in which atoms are in metastable positions, an important consideration for a highly disordered system. An "energy kill" process has been added to speed convergence to an equilibrium configuration and thereby reduce the computer time required. The concepts and terms which appear in this paragraph will be described and defined more fully in the following sections.

METHODS OF COMPUTER EXPERIMENTATION

Equations of Motion

The movement of atoms in GRAINS is done through the equations of motion, based on classical Newtonian mechanics, and the integration scheme developed by Gibson et al. (1960). Given a number of atoms (N), each with three degrees of freedom, determination of the velocities and position of each would require the integration of $3N$ coupled differential equations. The uncertainties associated with the potential functions, and the impracticalities of a calculus of combinatorial events, suggests that a simple central difference procedure would produce accuracy consistent with the knowledge of the force law and permit solutions to be obtained in a reasonable amount of computer time.

The integration procedure is as follows:

The position of an atom at time t is $x_i(t)$, where i describes the i^{th} coordinate, and its velocity is $v_i(t)$. Thus, $i = 1, 2, 3 \dots 3N$ fully describes the motion and position of all atoms each with three degrees of freedom, in a three dimensional system. The force in the i^{th} degree of freedom depends upon the position of all other atoms at that time and is

$$F_i[x_i(t) \ . \ . \ . \ . \ x_{3N}(t)] \ . \quad (1)$$

Since, according to the relationship

$$F = ma,$$

the acceleration at time t of an atom along the i^{th} coordinate is

$$a_i(t) = \dot{v}_i(t) = F_i[x_i(t) \ . \ . \ . \ . \ x_{3N}(t)]m^{-1} \quad (2)$$

where m is the mass of the atom, its velocity is

$$v_i(t) = \dot{x}_i(t). \quad (3)$$

The preceding can be derived rigorously or defined. The integration procedure is to replace time derivatives with finite time intervals, so that

$$\dot{v}_i(t) \approx [v_i(t + \Delta t/2) - v_i(t - \Delta t/2)] \Delta t^{-1}, \quad (4)$$

and

$$\dot{x}_i(t + \Delta t/2) \approx [x_i(t + \Delta t) - x_i(t)] \Delta t^{-1} \quad (5)$$

Rearrangement of equations (4) and (5) and substitution of equation (2) into equation (4) give the equations for velocity (at half time steps), and position at integral time steps

$$\begin{aligned} v_i(t + \Delta t/2) \approx \Delta t \, m^{-1} F_i[x_i \cdot \cdot \cdot x_{3N}] \\ + v_i(t - \Delta t/2) \end{aligned} \quad (6)$$

and

$$x_i(t + \Delta t) \approx \Delta t \, v_i(t + \Delta t/2) + x_i(t). \quad (7)$$

Equations (4) and (5) depend upon a linear variation in velocity during the time interval (Δt). If this is true, extrapolation from a point is possible since the slope is known at the midpoint of the interval, and the extrapolation will be accurate within the limitation of the determination of the slope, which in this case depends upon the force law.

Since the positions of the atoms are known at a given time, the acceleration is also known at even increments ($t \pm n\Delta t$) according to equation (2). Velocities are calculated at "half time steps" ($t \pm n/2\Delta t$) to preserve accuracy.

The choice of the magnitude of the time step is critical to the accuracy of the program. If it is too large, equations (4) and (5) will be in substantial error, and subsequently equations (6) and (7) give inexact results. If Δt is too small, computer time becomes excessive. For these reasons, it may be advantageous to maintain the initialized value.

Conservation of Energy

Since no work is done to or by the computational cells considered, there must be a conservation of energy; that is, the Hamiltonian function should be constant with time:

$$T = \text{Kinetic energy} = \sum_{i=1}^{3N} \frac{m(v_i)^2}{2}; \quad (8)$$

$$V_i = \text{Potential energy} = - \sum_{i=1}^N \sum_{j=1}^{3N} F_{ij} [x_i \cdot \cdot \cdot x_{3N}] r(x_i x_{3N}), \quad (9)$$

where r is the separation distance between atoms; and for the cell,

$$V = \sum_{i=1}^N V_i, \quad (10)$$

Since $H = T + V$, then the conservation of energy $\partial H / \partial t = 0$ must be maintained.

In the course of this investigation, the kinetic and potential energies are calculated and tabulated at each time step. A summation is made (i.e., the Hamiltonian) and tabulated. Variance over 0.001% in the Hamiltonian causes termination of the computation, since the system is exhibiting instability which is probably due to an inappropriately large time step. A variation in the Hamiltonian function (total energy) is apparent in the example output (Appendix B). This is not due to a non-conservative system, but merely to the fact that the potential energy summation includes both movable and immovable atoms. The potential energy of the immovable atoms changes because of changes in position of movable atoms within the range of the potential function. The kinetic energy of these atoms, however, remains at zero since no movement (velocity) is permitted. Thus, we have two regions, the interior of the cell and the boundary. In the interior of the cell, energy is conserved. But in the boundary regions, no motion is allowed and the kinetic energy must be zero; $dT/dt = 0$. But the potential energy changes as the movable atoms change position relative to the fixed atoms, so $dV/dt \neq 0$. Therefore,

$$\frac{dH}{dt} \neq \frac{dT}{dt} + \frac{dV}{dt} \neq 0. \quad (11)$$

That is, energy cannot be conserved in this region. Program changes made at the writing of this report, which exclude the potential energy of the immovable atoms in computation of the Hamiltonian, result in total conservation of energy unless an instability exists and until an "energy quench" is performed.

Energy Dampening

A fully dynamic computer calculation is one in which the atoms move freely until an equilibrium configuration is finally reached. Without an energy loss mechanism, atoms will

vibrate around their equilibrium positions indefinitely. If the purpose of the experiment is to compute an equilibrium configuration and energy, convergence to an accurate solution can be accomplished by "freezing" the atoms when the kinetic energy of the system reaches a maximum.

According to the conservation of energy, the system must be at its lowest potential energy when the kinetic energy is the greatest. In principle, it should be possible to arrive at a solution very quickly. However, since the computation is performed with finite time steps, it would be entirely fortuitous if a computer time step coincided exactly with that precise point in time at which the kinetic energy reached its maximum, so attainment of a solution requires several "energy kills." (See Figure 1.)

FIGURE 1. Schematic Approach to Convergence--Computer Experiment Methods

This process of the quench of kinetic energy is the basis of the quasi-dynamic method of computer experimentation described by Gehlen et al. (1968), and is employed in GRAINS. In the procedure in the code, the atoms are not moved if the kinetic energy at a time step is less than that in the immediately preceding step. When this occurs, the velocity components of all atoms are set to zero and the kinetic energy is quenched. Actually, if the velocities were set to zero at that instant, the integration procedure would be violated, and errors would be introduced into the numerical analysis procedure since velocity, position and force would be set at the same time rather than having velocity computed at the midpoints of time intervals. Therefore, the method which is followed is to compute velocities for a pseudo $(t_R - \Delta t/2)$ time, which, when combined with the acceleration at t_R , gives a mean velocity of zero through the interval

$$(t, - \Delta t/2) \text{ to } (t_R + \Delta t/2), \quad (12)$$

where t_R is the time when the reset or quench is performed.

Units

The exact values of length, time, energy, and velocity, used in computer experiments in general, and those values concerned with crystalline behavior in particular are either very large or small; thus the input and output would be cumbersome, and potential computer underflows or overflows could occur. It is, therefore, very convenient to normalize the units according to a scale of practical numbers. The following physical quantities and their dimensions are involved in the computations. (See Table 1.) When performing the computer experiments, the unit of energy is chosen to be the electron volt; the unit of length, the half lattice constant; and the unit of mass is the atomic mass unit. The units for the other physical quantities are derived from these. The method and values are as follows:

TABLE 1. Dimensions and Units of Computer Experiment Variables

Quantity	Symbol	Dimensions	Basic cgs Units
Length (distance)	x	L	cm
Time	t	t	sec
Mass	m	M	g
Velocity	v	$\frac{L}{t}$	$\frac{cm}{sec}$
Momentum	mv	$\frac{ML}{t}$	$\frac{gcm}{sec}$
Force	F	$\frac{ML}{t^2}$	gcm/sec ⁻² or dyne
Energy	E, T, V, or H	$\frac{ML^2}{t^2}$	gem ² /sec ⁻² , dyne-cm, erg, eV

$$\begin{aligned}
 \text{Energy} &= 1 \text{ eV} = 1.602 \times 10^{-12} \text{ ergs} \\
 &= 1.602 \times 10^{-12} \frac{gcm^2}{set^2} - \frac{mv^2}{2}, \quad (13)
 \end{aligned}$$

and,

$$\text{since the unit of mass} = 1 \text{ amu} = 1.659790 \times 10^{-24} \text{ g}, \quad (14)$$

$$\begin{aligned}
 \text{unit velocity is } v &= \left(\frac{2E}{m} \right)^{1/2} = \frac{2 \times 1.602 \times 10^{-12}}{1.659790 \times 10^{-24}} \\
 &\approx 1.39 \times 10^6 \frac{cm}{sec}; \quad (15)
 \end{aligned}$$

$$\text{dimensionally, } v = \left[\frac{ML^2}{t^2} / M \right]^{1/2} = L/t; \quad (16)$$

$$\begin{aligned}
 \text{then the unit' of time is } t &= L/v = \frac{1.823 \times 10^{-8}^*}{1.39 \times 10^6} \\
 &= 1.31 \times 10^{-14} \text{ sec.} \quad (17)
 \end{aligned}$$

* The unit of length is the half lattice constagt of the host material. For y-iron at 910 °C, a/2 = 1.823 Å (Pearson, 2967)

The unit of time should be less than the inverse of the Debye frequency of the material studied. The Debye frequency is

$$\nu_m = \frac{k\theta}{h}, \quad (18)$$

where k = Boltzmann's constant = 1.380×10^{-16} ergs/°K

θ = Debye's temperature = 467 °K for γ -iron

(Gray, 1963)

h = Planck's constant = 6.62517×10^{-27} erg-sec.

Thus,

$$\nu_m = 9.726 \times 10^{-12} \text{ sec}^{-1}, \quad (19)$$

and

$$(\nu_m)^{-1} = 1.03 \times 10^{-13} \quad (20)$$

so the unit of time is less than 1/10 the inverse of the maximum Debye frequency.

The use of these normalized units in the computer experiments permits convenient preparation and analysis of the results. In preliminary experiments on the grain boundary studies, the unit time interval of $\Delta t = 1.3 \times 10^{-14}$ sec was found to maintain accuracy. As a comparison, Gehlen et al. used an initial time step of less than 1.7×10^{-14} in their dislocation studies. No improvement in accuracy was achieved when either $\Delta t = 0.1$ or $\Delta t = 0.5$ were used, rather the times required for solution increased by factors of 10 and 2, respectively.

Cell Boundary

The boundary chosen for the computational cell is extremely important to the validity of the calculations. The boundary must simulate an infinite crystal beyond the region which encompasses the stress and strain fields of the defect studied. The boundary must be constructed so that it will not influence the energy or positions of atoms within the

volume of the defect strain field. The boundary must also preserve the crystallinity of the material studied, maintaining the structure and lattice constant.

Two types of boundaries are used in the cells constructed by GRAINS and in the calculations. These cells, which are rectangular parallelepipeds, have a mantle of fixed atoms on the four X-Z and Y-Z boundaries. The rigid mantle surrounding the cell on these four sides comprises the simplest possible type of boundary. This type of boundary is used in GRAINS because large computational cells can be constructed due to the speed of the code and available storage of the IBM-360 and UNIVAC-1108 computers. With these cells, defects can be located at sufficient distances from the rigid boundaries so that there is no influence of the rigid boundary on the calculations. However, the calculations must be monitored continually to ensure that there is no effect caused by the boundary.

The influence of the rigid boundaries on the computer experiments performed with GRAINS is monitored by computing and printing the potential energy of the boundary atoms at each time step. This energy summation is very sensitive to perturbations which the boundary causes, since very little strain on the atoms near the boundary is required to appreciably alter their energy. Typically, in a cell containing about 1200 atoms and having an energy of approximately 1500 eV, a change in the boundary energy of greater than 0.001 eV, following the introduction or movement of a defect, is considered to be unacceptable, and the cell size is increased. Changes on the order of 0.0003 eV or less are acceptable. Thus, calculations of formation or migration energies to accuracies of ± 0.005 eV are not influenced by the boundaries. Immobile atoms are designated with TAG = 1 in the printed output and as squares in plotted output. During the calculational routines, these atoms are treated as all others; their interactions with movable atoms

and other immovable atoms are computed in the same manner as movable-movable atomic interactions. Potential energies (bonds), forces and velocities are calculated, however, movement of TAG = 1 atoms is precluded by a logic branch of the program.

The periodic boundary conditions imposed on the X-Y faces of the computational cell mean that atoms on those planes are allowed only two degrees of freedom (i.e., no motion in the Z direction is permitted). The computational cell is constructed with the X-Y planes as frontal planes with succeeding planes in the direction repeating in accordance with the crystallographic system. Thus, every other (100) plane is identical. The grain boundaries studied in the experiments were tilt boundaries and therefore had their axis of rotation in the plane of the boundary. The axis of rotation was $\langle 100 \rangle$ and the boundaries were in a (010) plane. The grain boundary therefore sliced through the cell on a (010) plane and was considered infinite in the $\langle 010 \rangle$ and $\langle 001 \rangle$ directions.

Similarly, the edge dislocations studied were the (111), $\langle 110 \rangle$ slip system in which the dislocation extends normal to (112) planes. For these cases, the frontal planes are (112) planes and every sixth plane is identical.

This concept of periodicity is based on the premise that image planes will permit simulation of a crystal of infinite extent in a finite computational cell. This is acceptable for an extended defect, provided that the depth (i.e., number of planes along the Z axis) of the cell is at least an integral multiple of the repeat distance of the crystallographic system. For point defects studied alone, or in conjunction with these extended defects, the depth of the cell has to be sufficient to enclose the strains (u_i) induced by the defects. Thus, the depth of the computational cells was increased for these

studies and was invariably an odd multiple of the repeat distance, so that symmetry existed about the center (X-Y) plane into which the defects were introduced.

Atomic Interaction Functions

The accuracy of the functions used to determine the interaction between atoms is essential to the success of a computer experiment. The functions which were employed in this investigation are called interatomic functions rather than potential functions, since they are computed from experimental measurements of chosen properties of the material studied rather than being derived from first principles. They permit conservations of these properties, in this case the elastic constants, rather than striving to completely describe the potential functions within a lattice. Thus, they permit solution of complex many-body problems by summation of pairwise interactions with the accuracy of the data used to derive the function.

The assumption of the adequacy of the short range potentials, used in this study, is based upon the cell boundary constraint, simulating the volume effects felt in a lattice which exerts the cohesive forces necessary to maintain crystallinity. As a result, the local structure components of energy due to ion-ion interaction can be nonequilibrium in nature (i.e., either repulsive or attractive), since the cohesive volume forces, which are long range in nature, are simulated by a "pressure" on the surface of the cell.

Iron-Iron Function. The iron-iron interatomic function chosen for this study was that developed by Johnson (1966) originally for α -iron, the Johnson I potential. The first (R_1) neighbor position for γ -iron at 910 °C ($a = 3.646 \text{ \AA}$) is a nonequilibrium position, and the atoms feel a small repulsive force. The range of the potential does not include atoms in the

second neighbor positions, so the volume cohesive forces must be provided by surface pressure. The method of construction for this potential function is based upon the relations between the interatomic potential and the elastic constants, as derived by Fuchs (1936). The elastic constants define a parabolic potential function as a function of separation distance. Three cubic equations were chosen to give the potential. These are spline-fitted so that the functions and their first derivatives were continuous across the knots. The cut-off distance for the potential was arbitrarily chosen to be midway between the second and third neighbor distance for a-iron. The first of the cubics covers the range from very close separation to nearly the first neighbor distance, the second includes first and second neighbor distances in a-iron, and the third provides a smooth approach to zero energy at the cut-off distance. The analytical coefficients, used in the cubic equations describing the potentials used in GRAINS appear in Table 2.

TABLE 2. Interatomic Potential Functions Used in Grain Boundary Studies

Interatomic Distance, (r)		Coefficients			
	<u>Å</u>	<u>A</u>	<u>B</u>	<u>C</u>	<u>D</u>
<u>Iron-Iron-</u>					
0	to 2.40	-2.1959759	20.408808	-60.520588	57.851639
2.40	to 3.0	-0.63923	5.975194	-18.13981	17.754935
3.0	to 3.44	-1.115035	10.257440	-30.986551	30.601677
	>3.44	0	0	0	0
<u>Iron-Carbon</u>					
0	to 2.523	-3.365000	22.572420	-49.5859312	35.462413
	>2.523	0	0	0	0
<u>Carbon-Carbon</u>					
0	to 1.4	-4.763120	20.005102	-28.007143	13.0700
	>1.4	0	0	0	0

where $V = A(r)^3 + B(r)^2 + Cr + D$

Johnson (1966) points out that since the cohesive energy was not fitted to his interaction functions, formation energies calculated would be questionable because they are sensitive to the cut-off distance chosen. In fact, however, formation energies for vacancies calculated by Johnson (1966) and in this study agree quite well with experimental values. His conclusion, which appears correct, is that the short range potential based on elastic properties can give reasonable agreement with other physical properties, and that with such a semi-empirical potential it is questionable whether the minor effects arising from electronic contributions should be subtracted out.

Iron-Carbon Function. The interatomic function used for interactions between carbon impurity atoms and the host iron atoms, presented in Table 2, was also developed by Johnson (1965a). Upon obtaining values from the model which matched the experimentally determined values, construction of this function was based on the carbon migration energy (0.86 eV), the carbon-vacancy binding energy (0.47 eV), and the carbon migration activation volume ($r = 0$). This function was also developed using a spline-fitting technique and a trial and error procedure in which the slope of the function was varied until the above constants were obtained.

Carbon-Carbon Function. The function chosen to describe the carbon-carbon interactions is a simple, repulsive function developed by the authors. The necessity for a carbon-carbon function arose in studies of several types of impurities found in or near a grain boundary. The structure of the carbon inclusion was of secondary importance compared to its volume, which could be simulated using a properly chosen cut-off distance on a repulsive interaction function. The chosen cut-off distance was $1.40 \text{ \AA}$, twice the atomic radius for carbon as given by Slater (1964). The form of the function is a cubic since this is amenable to the code. No attempt was made in

the construction of this function to determine whether carbon atoms would assume a graphitic or diamond structure, thus the carbon atoms are treated as hard spheres in their totally repulsive interactions. The coefficients for this cubic function also appear in Table 2.

Recently, Abrahamson (1969) has suggested parameters for Born-Mayer type potentials based upon the Thomas-Fermi-Dirac approximation. His model for carbon-carbon interactions is

$$U(r) = A \exp(-br) \quad R_1 \leq R \leq R_u \quad (21)$$

where $A = 1316 \text{ eV}$, $b = 3.80959(\text{\AA})^{-1}$, $R_1 = 0.52917 \text{ \AA}$, and $R_u = 1.58751$. This would give a more energetic repulsion to carbon atoms than was considered advisable in computer experimentation. Since the primary objective of the function is to treat the carbon-carbon interactions as billiard balls, the cubic function based upon the lesser repulsive force and shorter range interaction was chosen.

GRAINS COMPUTER CODE

General Description

The purpose of this section of the report is to describe some of the techniques and functions of the program so that the calculated results can be analyzed and interpreted more knowledgeably. A listing of the program is presented in Appendix A, and a simplified flow chart is shown in Figures 2 and 3.

GRAINS is a computer code developed to study point or extended defects in crystals, using the quasi-dynamic method of computer experimentation. It is written in FORTRAN V (FORTRAN IV, Level H) and was originally used on the IBM-360 computer at North Carolina State University. That version of the program was also used on a UNIVAC-1108 computer.

FIGURE 2. GRAINS Program Flow Chart

FIGURE 3. GRAINS Program Flow Chart - Relaxation Routine

The fundamental check runs necessary to achieve and assure accuracy were made on both machines. These included tests of the computational routines to assure that atom movements and bond strengths were calculated exactly. Exhaustive comparisons were made with results from hand calculations to assure that no errors in the programming of these routines existed. Similarly, calculations of energy conservation and symmetry of strain around defects (vacancies and carbon interstitial impurity atoms) were made.

After the "checkout" was "largely" completed and the code was deemed ready for use, it was found that a number of local systems options, which would greatly reduce the running time and increase the convenience of preparing input as well as interpreting results, were available for use with the UNIVAC-1108. As a result of this usage, the program, as listed in Appendix A, will have to be modified if it is to be used at another installation. The principal addition to the code is the plotting routine. This routine, written for use with a CAL-COMP plotter, provides accurate graphical representation of the atomistic structure and is invaluable in analyzing data. Bad runs and mistakes can be recognized more readily and corrected. Structure or strain fields which would have been difficult or impossible to perceive from numerical data became immediately apparent when represented graphically. Important examples, include the structure of grain boundaries and the "healing" of grain boundaries with carbon atoms.

The other "local options" used involve manipulation, storage and retrieval of data on magnetic tapes, FASTRAND drums, (UNIVAC, 1966) and in the computer core. These are not only extremely convenient and fast, but permit complete reproduction of the results of a prior experiment, including positions, energies, and velocity components of each atom. This greatly speeds convergence and is essential for migration energy determinations.

As now dimensioned, the storage requirement for GRAINS is 47,467 decimal words; however, GRAINS can be used on a 32k computer if the plotting subroutine is deleted and the maximum number of atoms is reduced to 1500. Presently, a computational cell composed of 2500 atoms can be studied.

The computational speed of GRAINS is quite fast--the time required to reach an equilibrium configuration is approximately

proportional to the number of atoms. Originally, the computational routine comprised several subroutines. Although this simplified the development of the logic flow, we were still able to reduce the running time by 2/3 when the computational steps were included in the main program. Time savings were also achieved by streamlining the calculations of force and energies: e.g., in a cell with 1000 atoms, each atom can be tested against every other atom on each iteration and 3,000,000 force and velocity components calculated at each time step, but this figure is cut down to about 20,000 through the procedures developed.

The capabilities of GRAINS, listed in Appendix A, are as follows:

- (1) Setup at the following crystal structures with any chosen lattice constant:
 - fcc (100)
 - fcc (110)
 - fcc (111)
 - fcc (112)
 - bcc (100)
 - bcc (110)
- (2) Construction of a **tilt** boundary of any angle in any of these crystallographic systems.
- (3) Addition of up to 20 impurity or interstitial atoms at any position within the cell.
- (4) Simultaneous removal of any atom, or up to 50 atoms, to create vacancies or vacancy complexes.
- (5) Simultaneous movement of any atom, of any type, or up to five atoms, to any position in the cell.
- (6) "Freezing" of any atom, or up to five atoms, in any one, two or three degrees of freedom, or all atoms completely, for a specified number of time steps or for the duration of the calculation. This is the NIX routine, which is necessary in determining migration energies and paths.

- (7) Creation of single or several edge dislocation(s) according to the procedure developed by Cotterill and Doyama (1966).
- (8) Movement of all the atoms in a cell containing a dislocation to positions dictated by either isotropic or anisotropic elasticity theory. Thus, in the study of a dislocation, the cell boundary exactly simulates the elastic continuum provided it is at a distance far enough from the dislocation core to be in a region where elasticity theory is valid (i.e., where the atom displacement is less than 0.1% of the lattice constant). For complete solution of a dislocation configuration, the atoms within the cell are then relaxed to equilibrium positions.
- (9) Simulation of complete or partial dislocation.
- (10) Creation of a free surface for any of the crystallographic systems. This surface, which is unrestrained, can be used to study the behavior of defects near, in or on a free surface or void.

Data can be printed and/or plotted after exercising any of these options, if desired. The cell can then be "relaxed" to its equilibrium configuration, and the process repeated again if required.

Input/Output

The NAMELIST routine (available in FORTRAN programming) is used for the GRAINS input. This routine permits extreme flexibility in the preparation of input by eliminating the need for a specified order, number, and field length of input variables. Thereby, this eliminates a major source of errors and wasted time and provides a considerable measure of convenience. Input variables whose values are not often changed during a series of runs (e.g. the lattice constant, the atomic weight of the host material, etc.), but which should be retained as variables, can be initialized, or assigned values which will be used unless

changed by an input entry. The total input required for many, fairly complex studies often consists of less than 10 input entries which can be arranged in any order. A list of the NAMELIST variables and (where appropriate) their initialized values appears in the program listing (Appendix A).

Runs can be initiated in several ways:

- (1) Begin from data on input cards (from scratch)
- (2) Begin from data stored on magnetic tape to
 - (a) Continue iterating to a more complete solution
 - (b) Introduce defects
 - (c) Move atoms (host or impurity)
- (3) Begin a new case from data stored in core memory. Any of the program options can be exercised. Thus, an experiment can be conducted, the output tape prepared, and a new case begun while the data are retained in the core. Retrieval time is reduced to zero and complete detail is retained.
- (4) Begin from data on FASTRAND drum (UNIVAC, 1966). Retrieval time is much less than that for tape.

Throughout the course of this discussion, in the listing and in the tabulated output, the coordinate system is standard and does not refer to the Miller indices of the crystallographic system. The frontal plane of the computational cell is an X-Y plane. At this surface, the Z axis extends into the cell from $Z = 1$ at this surface. This is also the manner in which the planes are presented in the graphical output prepared by the computer. The relationship between the X, Y, and Z axes and the Miller indices depends upon the system constructed. Examples are:

<u>Frontal Plane</u>	<u>Direction of Axes</u>		
	<u>X</u>	<u>Y</u>	<u>Z</u>
(100)	$\langle 010 \rangle$	$\langle 001 \rangle$	$\langle \bar{1}00 \rangle$
(110)	$\langle \bar{1}10 \rangle$	$\langle 010 \rangle$	$\langle \bar{1}10 \rangle$
(111)	$\langle \bar{1}10 \rangle$	$\langle \bar{2}11 \rangle$	$\langle 11\bar{1} \rangle$
(112)	$\langle \bar{1}12 \rangle$	$\langle 111 \rangle$	$\langle 110 \rangle$

Translation of the axes for each system was discarded as being too cumbersome and a source of errors. In all systems, the axes are the same and the units are half-lattice constants.

A sample output appears in Appendix B. This consists of a tabulation of the values of the input variables and values of the following at each time step (i.e., iteration):

- The "time" in unit time steps
- The potential energy of the cell, which is a summation of the energies of all the atoms, both movable and immovable
- The total kinetic energy of the cell (eV)
- The number and energy of the atom with the greatest kinetic energy
- The sum of the potential energies of the immovable atoms
(Units of energy are electron volts)

The number of movable atoms, the total number of atoms, the average energy of these atoms, and finally the configuration energy, then appear in the output. The configurational energy is simply the difference between the potential energy of the cell on the first and last time steps.

At this point in the output, appropriate termination messages will appear if the run was stopped because a termination condition occurred. Convergence is the most frequent cause of termination. Other possible causes of termination are instability and oscillation. The computation is considered unstable if the kinetic energy increases 1% in a time step. If the potential energy increases by 5% or more, the computation is assumed to be in a blowup condition and the job is terminated immediately. If the potential energy of the cell oscillates three times, the limiter is reduced from $0.4 \text{ } a/2$ to $0.05 \text{ } a/2$. If oscillation occurs three more times, the program is terminated. The full output is printed and may be written on tape for any of these terminations, except for potential energy blowup.

Finally, an array is printed, which includes the number and position (in rectangular coordinates in units of $a/2$ half lattice constants) of each atom in the cell. Atom number 1 is always located at 1, 1, 1. Its mobility designation is TAG, where:

- 0 = Three degrees of freedom--completely movable
- 1 = Immovable
- 2 = Two degrees of freedom--no motion in X allowed
- 3 = Two degrees of freedom--no motion in Y allowed
- 4 = Two degrees of freedom--no motion in Z allowed.

Kind denotes the type of atom or site:

- 1 = Fe
- 2 = C
- 77 = vacancy

These data can also be written on magnetic tape since data storage is complete and convenient. It is essentially impossible to lose data from a run if an output tape is assigned, since an input variable, NMIN, sets the number of minutes the computer will be allowed to run. One minute before this time, the program will exit at the completion of an iteration and write a tape. Thus, if there is not sufficient time allowed to complete the printed output or plot tape, these data can be recovered from the output tape in just a few seconds. This is particularly important since often a series of jobs are run together to comprise a fairly long run. Costs are such that the loss of output would be unacceptable.

Construction of a Lattice Structure

The construction of a lattice is performed in the CUBE subroutine. The type of structure and frontal plane desired [e.g. fcc (100)] must be specified. The program then begins at position 1, 1, 1 and places atoms at the appropriate

positions. When the cell has been constructed to the chosen size, atoms within the range of the potential functions of the X-Z and Y-Z surfaces are designated as immovable.

Construction of a Tilt Boundary

The method of construction of a **tilt** boundary is simple but should be documented. A **tilt** boundary is one in which the axis of rotation lies within the plane of the boundary and therefore, for these studies, is parallel to the Z axis. The angle ϕ is the angle between the boundary plane and the mean [100] direction of the two grains; in this construction, it is 90°.

The most important parameters in the construction of a grain boundary in a computation cell are accurate simulation and conservation of:

- The lattice structure of both grains
- The appropriate alignment between grains
- The proper distance between grains
- The shape and size of the computational cell, so that irregularities in the cell boundary do not perturb the results.

The method finally developed consists of first constructing the left grain, grain A, and then superimposing a larger grain over it in such a way that the required size of the cell containing a grain boundary is obtained (Figure 4). Atoms from the second grain are rejected if:

- (1) They lie outside the boundaries of the cell to be constructed
- (2) They lie within the volume of the first grain
- (3) They are too close to atoms in the first grain constructed.

(Refer to shaded areas in Figure 4.)

Rejection of atoms which violate principles (1) or (2) is quite simple since these criteria are precisely defined; however

distance from the cell boundary to the grain boundary--particularly for a high angle of rotation. The overlay method sets up a pseudo-origin (xcor, ycor) on each X-Y plane and a grain of sufficient size to circumscribe the grain which is to be used in the computer experiment. The geometry and algebra are very straightforward; however, test cases were run with $\theta = 0^\circ$ and $\theta = 90^\circ$ to insure that a perfect crystal was obtained with the proper number and position of atoms. Although the scheme was very simple, a number of corrections and refinements in the arithmetic and programming were found to be necessary. Subsequently, a large number of grain boundaries with various angles of rotation and crystallographic systems were constructed.

Upon construction of the cell containing a grain boundary, which requires that a number of atoms be rejected according to the three criteria listed, the remaining atoms in grain B are numbered sequentially, beginning with the atom with the minimum X, Y, and Z coordinates and the number immediately following that of the atom having the maximum X, Y, and Z coordinates in grain A. Thus, the numbering sequence proceeds through grain A, and then grain B, without gaps. No attempt has been made to synthesize a system through which the neighbors (1st, 2nd, . . .) of an atom could be identified, since the concept of neighbor shells loses meaning near the extended defects studied.

Reject Study

As previously discussed, one of the most important foundations for a computer investigation on grain boundaries is the proper matching of the grains. The distance between them is critical since if it is too little, the grains will be in compression, and of course, in tension if the distance is too large. These forces arise because of the rigid boundaries of

the computational cells. Since these cannot relax, stresses normal to Y-Z surfaces of the movable atoms result, and non-equilibrium configurations would occur upon relaxation of the atoms.

The method of determining the correct intergranular spacing was to introduce a variable, REJ, into the program, which sets the minimum interatomic distance between atoms across the grain boundary. A series of computations, in which cells containing grain boundaries (6°) were constructed, were then made. These cells were identical except for a variation in the value of REJ. The energy of these cells was determined, and the value of REJ which gave the lowest energy, most negative, configuration could be assumed to be correct. The values chosen for REJ ranged from 1.2 to 2.0, the units being half lattice constants. The REJ value of 1.2 constitutes the nearest approach of atoms (without melting) in a split-interstitial configuration (Christian, 1965). The range of the potential function (Johnson I) is $3.44 \text{ \AA}$, or about 1.88 half lattice constants. Hence, the value $\text{REJ} = 2.0$ represents two opposing free surfaces which must "bow out" or deform to interact--clearly a high energy (tension) configuration. Data presented in Table 3 show there is a decided minimum of energy at $\text{REJ} = \sqrt{2}$, hence, this value for REJ was used in all further studies. Thus, if atoms in grain B are closer than $\sqrt{2} a/2$ to any atom in grain A, they are rejected. Atoms are retained which are exactly at the first neighbor distance. Upon the completion of this study, the value of REJ was initialized by a statement in the program and thus has a value of $\sqrt{2}$ half lattice constants for all computations, unless the investigator specifically chooses to change it.

A study was also conducted to determine the proper value of REJ for cells placed under a high pressure, which was simulated by reducing the value of the lattice constant. A more exhaustive study was conducted to determine the proper value for REJ under this somewhat unique situation, but again,

TABLE 3. Data on Studies Conducted to Optimize Intergranular Spacing of γ -Iron

REJ	Average Energy of Movable Atoms, $-E$ (eV)	Configurational Energy, $-E$ (eV)
1.2	0.989	474.253
1.35	0.991	477.868
1.414	0.993	477.993
1.45	0.985	476.045
1.60	0.997	475.197
1.80	0.961	472.060

$$a = 3.646 \text{ \AA}$$

the low energy configuration was that at $REJ = \sqrt{2}$. Data from these experiments are presented in Figure 5. A few, similar tests were made for 50° boundaries to eliminate doubt as to the correctness of the construction of high angle boundaries. The results were the same.

FIGURE 5. REJ Optimization Study

Checkout Analyses

Exposition of the detailed checks that an investigator should make on his equipment, which in this case is the computer code, may seem trivial and unnecessary to many readers. However, in a comprehensive report of this nature, it seems appropriate to include some mention of a few of the checks made, so that persons contemplating such a study can be aware of pitfalls, and those using the results of this investigation can evaluate the results more adequately. A basic trap in the preparation and use of a large, complex computer code is to assume that the cases are too complex to check with any other method and to place complete reliance and trust in the computer and its programming. This is a poor assumption, and it is necessary to verify all possible parameters by hand calculation and analyze cases which are tractable by means other than with the use of a large computer. The results are often surprising and always enlightening.

The most fundamental routine in the GRAINS program is the treatment of the equations of motion. Correct calculation of the forces on the atoms, and subsequently their velocities, positions and energies, is the basis of the entire analysis. Particularly, programming and logic errors in these routines cannot be tolerated. The following tests were made to achieve and assure accuracy:

- (1) A perfect crystal was set up and the atoms relaxed. No movement of the atoms should occur, the movable atoms should have identical energies, and the run should terminate immediately because of no energy variations between time .steps. The energy of the atoms must agree exactly with that obtained using the first neighbor distance in the equations defining the potential function. An atom has 12 first neighbors in an fcc lattice, and since each bond is shared between two

atoms, the potential energy of each atom within a perfect fcc crystal must be, for a potential which includes only first neighbors,

$$E = 12 V_i(r_1)/2. \quad (22)$$

- (2) Set up a case with only two movable atoms. These atoms must move to a separation distance which is at the minimum equilibrium position of the potential, and each must have a potential energy which is exactly one-half that specified by the function. The equilibrium position is the minimum of the curve, where

$$\frac{dV_i}{dr} = 0 = F_i(r_e). \quad (23)$$

Atoms which are placed closer together than r_e must obviously move away from each other, those placed too far apart must move inward, and those whose separation exceeds the range of the potential must remain motionless. This series of runs proved to point out several errors in signs and variable subscripting, which would probably have gone undetected much longer if these simple cases, in which one knew the correct answers, had not been run. The rate of convergence of these cases, i.e., the number of iterations necessary to completely stop oscillation about the equilibrium position, was very helpful in refining the "energy kill" routine, and in determining the proper time step Δt and the appropriate value for the limiter. The limiter ALIM is a term which specifies the maximum distance which an atom can move in any single "jump" or time interval and is intended to keep the cell from disintegrating if atoms

are placed at close separation distances. The value of ALIM is normally 0.4 half lattice constants. If the computer distance

$$x_i = v_i t \quad (24)$$

exceeds ALIM, the velocity is scaled down so that 0.4 hlc is the distance moved.

- (3) Run a case backward in time to determine cumulative integration errors. Errors are cumulative in the dynamic calculation.

Each of these preliminary analyses, or check runs, was performed before the analysis of grain boundary problems was made initially, and most of the were performed again after major modifications were made in the code.

ACKNOWLEDGMENTS

R. E. Dahl wishes to express his appreciation to Dr. R. S. Paul and the staff of the Battelle Seattle Research Center for aid and assistance which made timely publication of this work possible.

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APPENDIX A

GRAINS COMPUTER CODE LISTING

•

4. ELT CRSTL,7,690508, 20079

```

000001      KST* FCOPY
000002      COMMON AR(12548), TXVEL(2500), TYVEL(2500), TZVEL(2500), JMOV(2500
000003      1), POT(2500), IBUF(2000), ALIM, MAX, LAX, IPRINT, PERTRB, VAC, NIX
000004      2, RESET, SUREN, PCTEGY, KINEGY, TIME, ENERGY, VAXNIX, TIMNIX, PASS
000005      3, PERTIM, UNNIX, CELTIM, TXFOR, TYFOR, TZFOR, N(300), K1(300), S5H
000006      4, Y1(300), Z1(300), RFEC(3), RFEFE(3), RCC(3), CCFE(12), CFEFE(12)
000007      5, RCC(12), RFE, WC, VVAC, NVAC(50), ADATM(20,4), MADATM, C(12), S5
000008      6, R(3), INIX(50), AMOVE(5,3), HOSTPF, HOSTWT, HLC, NIXX(50), ENMAX
000009      7, NIXY(50), NIXZ(50), MOVE(5), LMOVE, MMOVE, REJ, C11, C12, XDISPL
000010      8, C44, PR, ISO, YDISPL, YDISP2, LDISL, LSTACK, LPART, PLTXZ, PLTLU
000011      9, NPL, NPU, TITLE(28), IDENT(28), LACP
000012      C
000013      DIMENSION X(2500), Y(2500), Z(2500), IMOV(2500), KIND(2500),
000014      1 DUMVAR(20)
000015      C
000016      EQUIVALENCE (AR(1),MAXNEW),(AR(2),RMOV),(AR(3),NCUB),(AR(4),LBCC),
000017      1(AR(5),MAX1),(AR(6),GRAIN),(AR(7),FREES),(AR(8),G),(AR(9),DEG),
000018      2(AR(10),CLAT),(AR(11),I2),(AR(12),J2),(AR(14),AI2),(AR(15),AJ2),
000019      3(AR(16),AK2),(AR(17),AIC),(AR(18),AJC),(AR(19),AKC),(AR(20),ADD),
000020      4(AR(21),LINT),(AR(22),INT1),(AR(23),XCON),(AR(24),YCON),(AR(25),
000021      5 ZCON),(AR(26),XMXX),(AR(27),YMYX),(AR(28),ZMXZ),(AR(13),K2),
000022      6(AR(29),X(1)),(AR(2529),Y(1)),(AR(5029),Z(1)),(AR(7529),DUMVAR(1))
000023      7,(AR(7549),IMOV(1)),(AR(10049),KIND(1)),(DUMVAR(1),QQ)
000024      C
000025      LOGICAL LBCC, FREES, LADD, LINT, ISO, GRAIN, IPRINT, LAX, PERTRB,
000026      1 ADD, VAC, NIX, RESET, HOSTPF, HOSTWT, LMOVE, LDISL, PLTXZ, LPART
000027      2, PLTLU, LSTACK
000028      C
000029      REAL VASS, KINEGY
000030      C
000031      INTEGER TITLE
000032      C
000033      END

```


GRAIN#1,69050R, 20092

```

000001      C      PROGRAM TO SET UP A GRAIN BOUNDARY IN A CRYSTAL AND CALCULATE THE
000002      C      LOWEST ENERGY POSITIONS FOR THE ATOMS THROUGH A QUASI-DYNAMIC
000003      C      COMPUTER EXPERIMENT
000004      C      NAMELIST INPUT (HAS THE FORM VAR1=1.3,VAR2=3.1,VAR3=.13,ETC.) ALL COLUMNS
000005      C      OF THE CARD MAY BE USED EXCEPT THE FIRST COLUMN OF EACH
000006      C      CARD, WHICH IS NOT READ BY NAMELIST.
000007      C
000008      C      I2      - MAXIMUM NUMBER OF PLANES IN THE X-DIRECTION
000009      C      J2      - MAXIMUM NUMBER OF PLANES IN THE Y-DIRECTION
000010      C      K2      - MAXIMUM NUMBER OF PLANES IN THE Z-DIRECTION
000011      C      TSTOP   - MAXIMUM LATTICE TIME (TSTOP * 1.7936E-14 = REAL TIME)
000012      C      GRAIN   - (LOGICAL) IS A GRAIN BOUNDARY OR FREE SURFACE TO BE STUDIED?
000013      C      G        - LOCATION OF GRAIN BOUNDARY OR FREE SURFACE ON X-AXIS
000014      C      DEG      - DEGREES OF ROTATION OF RIGHT HALF OF CRYSTAL TO FORM GRAIN
000015      C                      BOUNDARY
000016      C      FREEFS  - (LOGICAL) IS A FREE SURFACE TO BE STUDIED?
000017      C      NCUH    - CONFIGURATION OF CUBE (ORIENTATION OF X,Y PLANES)
000018      C                      FCC:      (INITIALIZED TO 100)
000019      C                      1 OR 100 GIVES (100) ORIENTATION
000020      C                      2 OR 110 GIVES (110) ORIENTATION
000021      C                      3 OR 111 GIVES (111) ORIENTATION
000022      C                      4 OR 112 GIVES (112) ORIENTATION
000023      C                      BCC:      (INITIALIZED TO 100)
000024      C                      1 OR 100 GIVES (100) ORIENTATION
000025      C                      2 OR 110 GIVES (110) ORIENTATION
000026      C      LAX      - (LOGICAL) SHOULD CRYSTAL BE RELAXED? (ITERATED UPON)
000027      C                      INITIALIZED TO TRUE
000028      C      PERTRB  - (LOGICAL) WILL LATTICE HAVE ANY DEFECTS (OTHER THAN GRAIN
000029      C                      BOUNDARY OR EDGE DISLOCATION) INTRODUCED? (VACANCIES, FIXED
000030      C                      ATOMS, INTERSTITIALS, ETC.)
000031      C      VAC      - (LOGICAL) ARE VACANCIES INTRODUCED?
000032      C      NVAC    - NUMBER OF VACANCIES TO BE INTRODUCED
000033      C      NVAC    - ATOM NUMBERS WHOSE SITES ARE TO BE VACATED
000034      C      LADD     - (LOGICAL) ARE INTERSTITIALS ADDED?
000035      C      NADATM   - NUMBER OF INTERSTITIAL ATOMS ADDED
000036      C      ADATM   - COORDINATES OF ADDED ATOMS      ADATM(1,1)=X-COORDINATE
000037      C                      ADATM(1,2)=Y-COORDINATE
000038      C                      ADATM(1,3)=Z-COORDINATE
000039      C                      ADATM(1,4)=ATOM TYPE
000040      C                      TYPE 1 = MAJOR ATOM TYPE
000041      C                      TYPE 2 = MINORITY ATOM TYPE
000042      C      LMVCE    - (LOGICAL) ARE ANY ATOMS TO BE DISPLACED?
000043      C      NMVCE    - NUMBER OF ATOMS TO BE MOVED
000044      C      MOVCE    - ATOM NUMBERS OF MOVED ATOMS

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00n045 C  AMOVE - NEW COORDINATES OF MOVED ATOMS
00n046 C  NIX - (LOGICAL) ARE ANY ATOMS TO BE FIXED?
00n047 C  MAXNIX - NUMBER OF ATOMS TO BE FIXED
00n048 C  INIX - ATOM NUMBERS WHICH HAVE ALL COORDINATES FIXED
00n049 C  NIXX - ATOM NUMBERS WHICH HAVE X-COORDINATE FIXED
00n050 C  NIXY - ATOM NUMBERS WHICH HAVE Y-COORDINATE FIXED
00n051 C  NIXZ - ATOM NUMBERS WHICH HAVE Z-COORDINATE FIXED
00n052 C  TIMNIX - LATTICE TIME WHEN ATOMS WITH ALL COORDINATES FIXED ARE RELEASED
00n053 C  NOTE: ONLY THOSE ATOMS WHICH HAVE ALL COORDINATES FIXED WILL
00n054 C  BE RELEASED AT TIME = TIMNIX
00n055 C  LINT - (LOGICAL) ARE THERE INTERSTITIALS ALREADY IN THE LATTICE BEING
00n056 C  READ IN FHGF TAPE?
00n057 C  INT1 - ATOM NUMBER OF FIRST INTERSTITIAL IF LINT IS TRUE
00n058 C  PERTIN - NUMBER OF TIME-STEPS TO BE RUN AFTER LATTICE IS PERTURBED
00n059 C  (TSTOP = TSTOP + PERTIN)
00n060 C  DELTIM - TIME-STEP INTERVALS (MAY BE WHOLE NUMBERS OR FRACTIONS)
00n061 C  INITIALIZED TO 1.0
00n062 C  ALIM - MAXIMUM DISTANCE ANY ATOM MAY MOVE IN ANY ONE TIME-STEP
00n063 C  INITIALIZED TO 0.4
00n064 C  LHCC - (LOGICAL) SHOULD A FCC LATTICE RATHER THAN AN FCC BE USED?
00n065 C  WFE - ATOMIC MASS OF MAJOR ATOM TYPE INITIALIZED TO 58.69 (NICKEL)
00n066 C  WC - ATOMIC WEIGHT OF TYPE 2 ATOM INITIALIZED TO 12.0 (CARBON)
00n067 C  REU - DISTANCE (HALF-LATTICE UNITS) OF CLOSEST APPROACH OF ATOMS
00n068 C  ALONG A GRAIN BOUNDARY INITIALIZED TO SQRT(2.)
00n069 C  CLAT - LATTICE CONSTANT (ANGSTROMS) INITIALIZED TO 3.646 (NICKEL)
00n070 C  LDISL - (LOGICAL) SHOULD AN EDGE DISLOCATION BE INTRODUCED?
00n071 C  ISO - (LOGICAL) IS THE DISPLACEMENT OF ATOMS AROUND THE DISLOCATION
00n072 C  CORE ISOTROPIC? INITIALIZED TO TRUE
00n073 C  C11 -\
00n074 C  C12 -- ELASTIC CONSTANTS FOR THE LATTICE INITIALIZED TO -/ 24.65
00n075 C  C44 -/ \ 12.47
00n076 C  PR - POISSON'S RATIO INITIALIZED TO 0.276
00n077 C  XDISPL - X-COORDINATE OF CENTER OF DISLOCATION CORE
00n078 C  YDISPL - Y-COORDINATE OF CENTER OF DISLOCATION CORE
00n079 C  LSTACK - (LOGICAL) ARE DISLOCATIONS TO BE STACKED TO SIMULATE A GRAIN
00n080 C  BOUNDARY?
00n081 C  YDISP2 - Y-COORDINATE OF CENTER OF LOWER DISLOCATION CORE IF LSTACK = T
00n082 C  LPART - (LOGICAL) SHOULD A PARTIAL RATHER THAN A COMPLETE DISLOCATION
00n083 C  BE CONSTRUCTED?
00n084 C  CFEFF - COEFFICIENTS OF CUBIC EVALUATION FOR POTENTIAL FUNCTION FOR
00n085 C  MAJOR ATOM TYPE (TYPE 1) INITIALIZED TO JOHNSON-I
00n086 C  (3 RANGES, 4 COEFFICIENTS EACH) ALPHA IRON OR NICKEL
00n087 C  RFEFF - END-POINTS OF RANGES FOR CFEFF INITIALIZED SAME AS CFEFF
00n088 C  CCFE - SAME AS CFEFF FOR INTERACTION BETWEEN TYPE 1 AND TYPE 2 ATOMS
00n089 C  INITIALIZED TO NICKEL-CARBON POTENTIAL
00n090 C  RFECL - END-POINTS OF RANGES OF INTERACTION POTENTIAL BETWEEN TYPE 1
00n091 C  AND TYPE 2 ATOMS INITIALIZED SAME AS FOR CCFE
00n092 C  CCC - SAME AS CFEFF FOR INTERACTION BETWEEN ATOMS OF TYPE 2
00n093 C  INITIALIZED TO CARBON POTENTIAL

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00n094 C RCC - RANGE ENDS FOR CCC INITIALIZED SAME AS CCC
00n095 C IPRINT - (LOGICAL) PRINT OUT UNRELAXED CRYSTAL?
00n096 C PLOT - (LOGICAL) IS THIS LATTICE TO BE PLOTTED?
00n097 C SAVE - (LOGICAL) IS THIS LATTICE CONFIGURATION TO BE SAVED ON TAPE?
00n098 C REPEAT - (LOGICAL) IS THE LATTICE CONFIGURATION TO BE READ FROM TAPE?
00n099 C REDC - (LOGICAL) IS THE RELAXED LATTICE FROM THE CASE IMMEDIATELY
00n100 C PRECEDING THIS CASE TO BE USED IN THIS CASE? (SAME RUN)
00n101 C LREP - (LOGICAL) SHOULD THE FILE JUST PROCESSED BE READ IN AS LATTICE
00n102 C FOR THIS CASE?
00n103 C LSETF - (LOGICAL) SHOULD THE INPUT TAPE BE CHANGED?
00n104 C NEFF - TAPE UNIT TO BE USED INSTEAD OF UNIT F INITIALIZED TO 12 (G)
00n105 C NFILEI - FILE NUMBER TO BE READ IN
00n106 C LPT - (LOGICAL) SHOULD THE NUMBER OF SECONDS PER ITERATION BE PRINTED?
00n107 C NFILEO - TAPE FILE TO BE WRITTEN UPON
00n108 C DELMAX - THE MAXIMUM FRACTIONAL CHANGE IN POTENTIAL ENERGY BETWEEN ANY
00n109 C TWO CONSECUTIVE TIME-STEPS INITIALIZED TO 0.05
00n110 C DELMIN - THE MINIMUM FRACTIONAL CHANGE IN POTENTIAL ENERGY BETWEEN ANY
00n111 C TWO CONSECUTIVE TIME-STEPS INITIALIZED TO 5.0E-6
00n112 C LAST - (LOGICAL) IS THIS THE LAST CASE IN THIS RUN?
00n113 C NMIN - NUMBER OF MINUTES (COMPUTER TIME) FOR WHICH THE RUN SHOULD GO
00n114 C PLTXZ - (LOGICAL) SHOULD PLOTS BE MADE OF (X,Z) PLANES?
00n115 C PLTLU - (LOGICAL) SHOULD SELECTED PLANES BE PLOTTED?
00n116 C NPL - NUMBER OF THE LOWEST PLANE TO BE PLOTTED
00n117 C NPU - NUMBER OF THE HIGHEST PLANE TO BE PLOTTED
00n118 C LINCIT - (LOGICAL) SHOULD THE BOUNDARY BE RELAXED AFTER THE CELL HAS
00n119 C ACHIEVED CONVERGENCE, AND THEN RE-RELAX THE CELL?
00n120 C
00n121 C THE UNIT OF LENGTH IS THE HALF LATTICE COESTANT (FOR NICKEL, L=1.762 E-P CM
00n122 C THE UNIT OF ENERGY IS THE ELECTRON VOLT ( 1EV=1.602E-12 ERGS(G*CM**2/SEC**2))
00n123 C THE UNIT OF MASS IS 1.0E-24 GRAMS
00n124 C THE UNIT OF TIME IS 1.7936 E-14 SECONDS
00n125 C THE UNIT OF VELOCITY IS 1.0179 E6 CM/SEC
00n126 C
00n127 C INCLUDE KST
00n128 C
00n129 C DIST(XX,A,YY,B,ZZ,C)=SQRT((XX-A)**2+(YY-B)**2+(ZZ-C)**2)
00n130 C
00n131 C DIMENSION JROG(2)/'READING'/, INTG(2)/'WRITING'/
00n13 C
LOGICAL S, L, L1, L2, L3, L4, L5, L6, L7, L8, L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20, L21, L22, L23, L24, L25, L26, L27, L28, L29, L30, L31, L32, L33, L34, L35, L36, L37, L38, L39, L40, L41, L42, L43, L44, L45, L46, L47, L48, L49, L50, L51, L52, L53, L54, L55, L56, L57, L58, L59, L60, L61, L62, L63, L64, L65, L66, L67, L68, L69, L70, L71, L72, L73, L74, L75, L76, L77, L78, L79, L80, L81, L82, L83, L84, L85, L86, L87, L88, L89, L90, L91, L92, L93, L94, L95, L96, L97, L98, L99, L100, L101, L102, L103, L104, L105, L106, L107, L108, L109, L110, L111, L112, L113, L114, L115, L116, L117, L118, L119, L120, L121, L122, L123, L124, L125, L126, L127, L128, L129, L130, L131, L132, L133, L134, L135, L136, L137, L138, L139, L140, L141, L142, L143, L144, L145, L146, L147, L148, L149, L150, L151, L152, L153, L154, L155, L156, L157, L158, L159, L160, L161, L162, L163, L164, L165, L166, L167, L168, L169, L170, L171, L172, L173, L174, L175, L176, L177, L178, L179, L180, L181, L182, 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00n144      C
00n145      CALL ETIME
00n146      C
00n147      C      INITIALIZATION OF COMMON INPUT PARAMETERS: DATA INPUT CAN OVERRIDE
00n148      C
00n149      DELTIM = 1.
00n150      CLAT = 3.646
00n151      NCUR = 100
00n152      CFEFE(1) = -2.1959759
00n153      CFEFE(2) = 20.408808
00n154      CFEFE(3) = -60.520588
00n155      CFEFE(4) = 57.851639
00n156      CFEFE(5) = -.63923
00n157      CFEFE(6) = 5.975194
00n158      CFEFE(7) = -18.13981
00n159      CFEFE(8) = 17.754935
00n160      CFEFE(9) = -1.115035
00n161      CFEFE(10) = 10.25794
00n162      CFEFE(11) = -38.986551
00n163      CFEFE(12) = 30.601677
00n164      RFEFE(1) = 2.4
00n165      RFEFE(2) = 3.0
00n166      RFEFE(3) = 3.44
00n167      CCFE(9) = -3.365
00n168      CCFE(10) = 22.57242005
00n169      CCFE(11) = -49.58593115
00n170      CCFE(12) = 35.4624127
00n171      RFEC(3) = 2.523
00n172      CCC(9) = -4.763119534
00n173      CCC(10) = 20.00510204
00n174      CCC(11) = -28.00714286
00n175      CCC(12) = 13.07
00n176      RCC(3) = 1.4
00n177      WFE=58.69
00n178      WC=12.0
00n179      REU = SQRT(2.0)
00n180      LAX = .TRUE.
00n181      DELMAX = 0.05
00n182      DELMIN = 5.E-6
00n183      NEFF = 12
00n184      FIRST = .TRUE.
00n185      SG2 = REU
00n186      SG22 = REU / 2.
00n187      (CON = 1.
00n188      (CON = 1.
00n189      ZCON = 1.
00n190      C11 = 24.65
00n191      C12 = 14.73

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00n192      C44 = 12.47
00n193      PR = 0.276
00n194      ISO = .TRUE.
00n195      NMIN = 10
00n196      LSI = .TRUE.
00n197      PERTIM = 100.
00n198      TSTOM=100.
00n199      NWC = 12548
00n200
00n201      C
00n202      1 FORMAT('1PERFECT CRYSTAL  (' , I3, ') ORIENTATION OF (X,Y) PLANES'
00n203      1      , //, ' (MOVABLE ATOMS ARE NOTED BY A TAG 0
00n204      2F 0; IMMOVABLE ATOMS BY A TAG OF 1)', //, 3(' ATOM NO.  X
00n205      3Y      Z      TAG      ', //)
00n206      2 FORMAT(3(I6, 3F9.2, 15, 5X))
00n207      3 FORMAT('0TOTAL ATOMS IN CRYSTAL WITH GRAIN BOUNDARY', I9, /
00n208      5      '0MOVABLE ATOMS IN CRYSTAL WITH GRAIN BOUNDARY', I7, /
00n209      6      '0LOCATION OF GRAIN BOUNDARY      X =', F9.4, /
00n210      7      '0ANGLE OF ROTATION' DEGREES      ', F15.8)
00n211      4 FORMAT(1X, I4, 3F15.6, 255, I11, 3F15.6, 215)
00n212      5 FORMAT(1X, I4, 3F10.6, F13.7, 215, I13, 3F10.6, F13.6, 215)
00n213      6 FORMAT('1CRYSTAL WITH GRAIN BOUNDARY:  (' , I3, ') ORIENTATION OF
00n214      1(X,Y) PLANES ', //, ' (MOVABLE ATOMS ARE DESIGNATED BY A TAG OF 0;
00n215      2IMMOVABLE ATOMS BY A TAG OF 1) //, Z(' ATOM NO.  X
00n216      3      Y      Z      TAG TYPE      ', //)
00n217      7 FORMAT('1CRYSTAL AFTER RELAXATION:  (' , I3, ') ORIENTATION OF
00n218      1(X,Y) PLANES ', //, ' (MOVABLE ATOMS ARE NOTED
00n219      2C BY A TAG OF 0; IMMOVABLE ATOMS BY A TAG OF 1)', //, 3(' ATOM
00n220      3 X      Y      Z      P.ENERGY TAG TYPE      ', //)
00n221      8 FORMAT(13A6, 1A2)
00n222      9 FORMAT('1', 9X, 'TIME', 12X, 'POTENTIAL ENERGY', 5X, 'KINETIC ENERGY', 6X
00n223      1, 'TOTAL ENERGY', 4X, 'MAXIMUM KINETIC ENERGY', 4X, 'SURFACE ENERGY (PO
00n224      2T)')
00n225      10 FORMAT('0ON THE LAST TIME STEP THE AVERAGE POTENTIAL ENERGY PER AT
00n226      1OM IS: ', 1PE15.7, ', AND THE TOTAL NUMBER OF ATOMS IS: ', I5,
00n227      2 / '0THE AVERAGE POTENTIAL ENERGY PER MOVABLE ATOM IS: ', 1PE15.7,
00n228      3, ' AND THE NUMBER OF MOVABLE ATOMS IS: ', I5 // '0CONFIGURATION EN
00n229      4ERGY = ', 1PE13.7)
00n230      11 FORMAT('// 0RUN TERMINATED BECAUSE THE TOTAL ENERGY CHANGE EXCEEDS
00n231      1 ', 0PF10.4, ', EDEL = ', F10.4, //)
00n232      12 FORMAT('// 0RUN TERMINATED BECAUSE TOTAL ENERGY CHANGE IS LESS TH
00n233      1AN', 1PE14.5, ', DELPOT = ', 1PE14.5, //)
00n234      13 FORMAT(1X, 0PF14.3, F25.6, 1PE20.7, 0PF19.6, 1PE17.7, ' (' , I14,
00n235      1 ')', 0PF19.6)
00n236      14 FORMAT(/, 25X, 13A6, 1A2)
00n237      15 FORMAT('1' //, 23X, '*****
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01060      823*****
01061      824*****
01062      825*****
01063      826*****
01064      827*****
01065      828*****
01066      829*****
01067      830*****
01068      831*****
01069      832*****
01070      833*****
01071      834*****
01072      835*****
01073      836*****
01074      837*****
01075      838*****
01076      839*****
01077      840*****
01078      841*****
01079      842*****
01080      843*****
01081      844*****
01082      845*****
01083      846*****
01084      847*****
01085      848*****
01086      849*****
01087      850*****
01088      851*****
01089      852*****
01090      853*****
01091      854*****
01092      855*****
01093      856*****
01094      857*****
01095      858*****
01096      859*****
01097      860*****
01098      861*****
01099      862*****
01100      863*****
01101      864*****
01102      865
```

```

000241      5**  * * * * * 1,20X 1***,12X 1 *** ** * * * * *
000242      6*  * * * * * 1,20X 1***,12X 1 *** ** * * * * *
000243      7**  * * * * * 1,20X 1***,12X 1 *** ** * * * * *
000244      8*  * * * * * 1,20X 1***,12X 1 *** ** * * * * *
000245      9*  * * * * * 1,20X 1***,12X 1 *** ** * * * * *
000246      *  * * * * * 1,20X 1***,12X 1 *** ** * * * * *
000247      1  * * * * * 1,20X 1***,12X 1 *** ** * * * * *
000248      2**  * * * * * 1,20X 1***,12X 1 *** ** * * * * *
000249      16 FORMAT(' SECONDS TAKEN FOR THIS ITERATION', I12 /)
000250      17 FORMAT('Q')
000251      C
000252      CALL SETEND(3HCSR, $117)
000253      C
000254      20 CALL SETECF($122 I
000255      READ(5, 8) TITLE
000256      WRITE(6,15)
000257      WRITE(6,14) °ITLE
000258      CALL SETNL(80I
000259      LDISL = .FALSE.
000260      GRAIN = .FALSE.
000261      ALIM = 0.4
000262      READ(5,NAM1)
000263      CALL SETNL(132)
000264      WRITE(6,NAM1)
000265      NS = (NMIN - 1) * 60
000266      IF(.NOT.PLOT.OR..NOT.FIRST) GO TO 21
000267      CALL CPLOTS(1BUF,2000,2)
000268      CALL CPLOT(1.0, 2.0, -3)
000269      FIRST = .FALSE.
000270      21 CONTINUE
000271      HLC = CLAT / 2.
000272      RESFT = .TRUE.
000273      CALL SETECF($36)
000274      IF(RFDO) GO TO 45
000275      IF(RFPEAT) GO TO 30
000276      A12 = I2
000277      A2 = J2
000278      AK2 = K2
000279      I = G + 0.01
000280      IF(.NOT.GRAIN) I = I2
000281      CALL CLBE(I, J2, 0)
000282      MAX1 = MAX
000283      IF(GRAIN.AND..NOT.FREES) CALL ROTATE
000284      MCV = 0
000285      K = 0
000286      GG = (RFEFE(3) + .01) / HLC + 1.
000287      IF(LDISL) CALL DISLOC
000288      IF(24 M=1,MAX
000289      IF(LDISL) GO TO 23

```

```

000290      IF(X(M).LT.WG.CR.Y(M).LT.QG.CR.X(M).GT.AIC.OR.Y(M).GT.AUC) GOTO 22
000291      IMOV(M) = 0
000292      NMOV = NMOV + 1
000293      GO TO 23
000294 22 IMOV(M) = 1
000295 23 CONTINUE
000296      IF(X(M).LT.W.) GO TO 24
000297      K = K + 1
000298      IMOV(K) = IMOV(M)
000299      X(K) = X(M)
000300      Y(K) = Y(M)
000301      Z(K) = Z(M)
000302 24 CONTINUE
000303      MAXNEW = <
000304      IF(GRAIN.OR.FREES) GO TO 28
000305      G = AIP 2.
000306      J = 0
000307      M = 0
000308      DO 26 I=1,MAXNEW
000309      IF(X(I).GT.G) GO TO 25
000310      M = M + 1
000311      X(M) = X(I)
000312      Y(M) = Y(I)
000313      Z(M) = Z(I)
000314      IMOV(M) = IMOV(I)
000315      GO TO 26
000316 25 J = J + 1
000317      TXVEL(J) = X(I)
000318      TYVEL(J) = Y(I)
000319      TZVEL(J) = Z(I)
000320      KIND(J) = IMOV(I)
000321 26 CONTINUE
000322      MAX1 =
000323      DO 27 I=1,J
000324      M = M + 1
000325      X(M) = TXVEL(I)
000326      Y(M) = TYVEL(I)
000327      Z(M) = TZVEL(I)
000328      IMOV(M) = KIND(I)
000329 27 CONTINUE
000330 28 DO 29 I=1,MAXNEW
000331      TXVEL(I) = 0.0
000332      TYVEL(I) = 0.0
000333      TZVEL(I) = 0.0
000334      POT(I) = 0.0
000335      KIND(I) = 1
000336 29 CONTINUE
000337      IF(SAVE) GO TO 33
000338      GO TO 45

```

```

00n339      30 IF(LREP) GO TO 35
00n340      IF(.NOT.LSETF) GO TO 31
00n341      CALL NTRAN(4,11)
00n342      CALL SETIO(4,NEFF)
00n343      31 IF(NFILEI.LE.1) GO TO 32
00n344      NFI = NFILEI = 1
00n345      CALL NTRAN(4,8,NFI)
00n346      32 IF(.NOT.SAVE) GO TO 36
00n347      33 IF(NFILEO.LE.1) GO TO 34
00n348      IF(.NOT.LS1) GO TO 34
00n349      NFO = NFILEO = 1
00n350      CALL NTRAN(3,8,NFO)
00n351      C
00n352      C      CHECK TO MAKE SURE TAPE 'B' PAS 4 RING 1A IT
00n353      C
00n354      WRITE(3,15)
00n355      CALL NTRAN(3,10)
00n356      CALL NTRAN(3,8,NFO)
00n357      LS1 = .FALSE.
00n358      NFILEO = 0
00n359      34 IF(REPEAT) GO TO 36
00n360      GO TO 45
00n361      35 CALL NTRAN(4,8,-1)
00n362      36 READ(4) IDENT
00n363      CALL NTRAN(4,2,NWD,AR,IVR)
00n364      IVR = IVR
00n365      WRITE(6,14) IDENT
00n366      37 IF(IVR.EQ.-1) GO TO 37
00n367      IF(IVR.LT.NWD) GO TO 124
00n368      IF(G.LT..01) G = A12
00n369      IF(LINOUT) LAX = .FALSE.
00n370      45 CONTINUE
00n371      IF(.NOT.IPRINT) GO TO 46
00n372      *WRITE(6,6) NCUB
00n373      WRITE(6,4) (M,X(M),Y(M),Z(M),IMOV(M),KIND(M),N=1,MAXNEW)
00n374      *WRITE(6,3) MAXNEW, NMOV, G, DEG
00n375      IF(PLOT) CALL GPLCT(MAXNEW)
00n376      46 CONTINUE
00n377      DO 47 I=1,12
00n378      C(I)=CFEFE(I)
00n379      47 CONTINUE
00n380      DO 48 J=1,*
00n381      R(J)=RFEFE(J)
00n382      48 CONTINUE
00n383      SS=(R(3)/PLC)
00n384      SSF = 55
00n385      VASS=*FE/1.66048
00n386      HCSIPF=.TRUE.
00n387      HCSINT=.TRUE.

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00n388      TIME=0.0
00n389      FL=0.0
00n390      LCEL = .FALSE.
00n391      ICCS = 0
00n392      LCSC = .FALSE.
00n393      IF(.NOT.LAX) GO TO 112
00n394      WRITE(6,9)
00n395      50 PCTEGY=0.0
00n396      KINEGY=0.0
00n397      ENERGY=0.0
00n398      SUREN=0.0
00n399
00n400      C
00n401      C      RELAXATION ROUTINE
00n402      C
00n402      FRMAX = 0.0
00n403      DO 95 M=1,MAXNEW
00n404      FCT(M)=0.0
00n405      IF(KIND(M).EQ.77) GO TO 95
00n406      FCRCE=0.0
00n407      TXFOR=0.0
00n408      TYFOR=0.0
00n409      TZFOR=0.0
00n410      IF(.NOT.ACD) GO TO 60
00n411      KII=KIND(M)
00n412      IF(KII.EQ.1.AND.HCSTWT) GO TO 60
00n413      GO TO (55,56,57,58,59), KII
00n414      55 MASS=WF/1.66048
00n415      FOSTPF = .FALSE.
00n416      HCSTWT=.TRUE.
00n417      GO TO 60
00n418      56 MASS=WC/1.66048
00n419      HCSTWT=.FALSE.
00n420      GO TO 60
00n421      57 CONTINUE
00n422      HCSTWT=.FALSE.
00n423      58 CONTINUE
00n424      HCSTWT=.FALSE
00n425      59 CONTINUE
00n426      HCSTWT=.FALSE.
00n427      60 CONTINUE
00n428      IF(X(M).LT.G-55H) GO TO 61
00n429      IF(X(M).GT.G+55H.AND..NOT.FRFES) GO TO 62
00n430      M1 = 1
00n431      M2 = MAXNEW
00n432      GO TO 63
00n433      61 M1 = 1
00n434      M2 = VAX1
00n435      GO TO 63
00n436      62 M1 = VAX1

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```

000437 M2 = MAXNEW
000438 63 DO 90 K=M1,M2
000439 IF (KIND(K).EQ.77) GO TO 90
000440 IF (ABS(X(M)-X(K)).GT.S5H) GO TO 90
000441 IF (ABS(Y(M)-Y(K)).GT.S5H) GO TO 90
000442 IF (ABS(Z(M)-Z(K)).GT.S5H) GO TO 90
000443 IF (M.EQ.K) GO TO 90
000444 D = DIST(X(M),X(K),Y(M),Y(K),Z(M),Z(K))
000445 IF (D.GT.S5H) GO TO 90
000446 IF (.NOT.ADC) GO TO 81
000447 IF (KIND(M).EQ.KIND(K).AND.HOSTPF) GO TO 81
000448 IF (KIND(M).NE.KIND(K).AND..NOT.HOSTPF) GO TO 81
000449 KI = KIND(M) + KIND(K) - 1
000450 GO TO (75,65,70), KI
000451 65 DO 66 I=1,12
000452 C(I)=CCFE(I)
000453 66 CONTINUE
000454 DO 67 J=1,3
000455 R(J)=RFEC(J)
000456 67 CONTINUE
000457 HOSTPF=.FALSE.
000458 GO TO 80
000459 70 DO 71 I=1,12
000460 C(I)=CCC(I)
000461 71 CONTINUE
000462 DO 72 J=1,3
000463 R(J)=RCC(J)
000464 72 CONTINUE
000465 HOSTPF = .TRUE.
000466 GO TO 80
000467 75 DO 76 I=1,12
000468 C(I)=CFEFE(I)
000469 76 CONTINUE
000470 DO 77 J=1,3
000471 R(J)=RFEFE(J)
000472 77 CONTINUE
000473 HOSTPF=.TRUE.
000474 80 SS=(R(3)/HLC)
000475 81 CONTINUE
000476 IF (.GT.S5) GO TO 90
000477 ANG=0*HLC
000478 A2 = ANG * ANG
000479 IF (ANG.LE.R(1)) GO TO 85
000480 IF (ANG.LE.R(2)) GO TO 86
000481 FBT=(C(9)*A2*ANG + C(10)*A2 + C(11)*ANG + C(12))/2.
000482 FCR = -(3.*C(9)*A2 + 2.*C(10)*ANG + C(11))
000483 GO TO 87
000484 85 FBT=(C(1)*A2*ANG + C( 2)*A2 + C( 3)*ANG + C( 4))/2.
000485 FCR = -(3.*C(1)*A2 + 2.*C( 2)*ANG + C( 3))

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00n486      GO TO A7
00n487      FBT = (C(5)*A2*ANG + C( 6)*A2 + C( 7)*ANG + C( 8))/2.
00n488      FCR = -(3.*C(5)*A2 + 2 *C( 6)*ANG + C( 7))
00n489      FD = FCR / B
00n490      TXFOR = TXFOR + (X(M) - X(K)) * FD
00n491      TYFOR = TYFOR + (Y(M) - Y(K)) * FD
00n492      TZFOR = TZFOR + (Z(M) - Z(K)) * FD
00n493      POT(M)=POT(M)+EPT
00n494      90 CONTINUE
00n495      IF(.NOT.ADD) GO TO 91
00n496      IF(N2.EG.MAXNEW) GO TO 91
00n497      M1 = INT1
00n498      M2 = MAXNEW
00n499      GO TO 63
00n500      91 PCTEGY = PCTEGY + POT(M)
00n501      IF(INCV(M).EQ.1) GO TO 94
00n502      DM = DELTIM / MASS
00n503      IF(.NOT.RESET)GO TO 92
00n504      D2M = -LM / 2.
00n505      TXVEL(M) = D2M * TXFOR
00n506      TYVEL(M) = D2M * TYFOR
00n507      TZVEL(M) = D2M * TZFOR
00n508      92 CONTINUE
00n509      TXVEL(M) = TXVEL(M) + TXFOR * DM
00n510      TYVEL(M) = TYVEL(M) + TYFOR * DM
00n511      TZVEL(M) = TZVEL(M) + TZFOR * DM
00n512      IF(Z(M).GT.AKC.CR.Z(M).LT.0.) TZVEL(M) = 0.0
00n513      VELOC2 = TXVEL(M)*TXVEL(M)+TYVEL(M)*TYVEL(M)+TZVEL(M)*TZVEL(M)
00n514      EMX = MASS * VELOC2 / 2.
00n515      KINEGY = KINEGY + EMX
00n516      IF(EMX.GT.ENMAX) IMAX = M
00n517      ENMAX = AMAX1(ENMAX,EMX)
00n518      DV = SQRT(VELOC2) * DELTIM
00n519      IF(DV.LT.ALIM) GO TO 93
00n520      SCALE = ALIM / DV
00n521      TXVEL(M) = TXVEL(M) * SCALE
00n522      TYVEL(M) = TYVEL(M) * SCALE
00n523      TZVEL(M) = TZVEL(M) * SCALE
00n524      93 IF(INCV(M).LT.2) GO TO 95
00n525      IF(INCV(M).EQ.2)TXVEL(M)=0.0
00n526      IF(INCV(M).EQ.3)TYVEL(M)=0.0
00n527      IF(INCV(M).EQ.4)TZVEL(M)=0.0
00n528      GO TO 95
00n529      94 SUREN = SUREN + PCT(M)
00n530      95 CONTINUE
00n531      ENERGY = KINEGY + PTEGY
00n532      IF(.RESET) GO TO 96
00n533      IF(KINEGY.LT.EL) GO TO 96
00n534      EL = KINEGY

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000535      DO 97 M=1,MAXNEW
000536      IF(INCV(M).EQ.1)GO TO 97
000537      X(M) = X(M) + IXVEL(M) * DELTIM
000538      Y(M) = Y(M) + IYVEL(M) * DELTIM
000539      Z(M) = Z(M) + IZVEL(M) * DELTIM
000540  97 CONTINUE
000541      RESET=.FALSE.
000542      GO TO 99
000543  48 RESET = .TRUE.
C
C      END OF RELAXATION ROUTINE
C
000547  99 WRITE(6,13) TIME, PTEGY, KINEGY, ENERGY, ENMAX, IMAX, SUREN
000548      IF(TIME) 102,
000549      EDL = ABS((ENERGY - ELAST) / ENERGY)
000550      IF (EDL.GT.DELMAX) GO TO 116
000551      IF(RESET) GO TO 100
000552      OLDPOI = ABS((PTEGY - OLDPOI) / PTEGY)
000553      IF(OLDPOI.LT.DELMIN) GO TO 105
000554      IF(OLDPOI.GE.PTEGY) GO TO 199
000555      ICCS = ICCS + 1
000556      IF(ICCS.LE.2) GO TO 199
000557      IF(LOSC) GO TO 204
000558      LOSC = .TRUE.
000559      ICCS = 0
000560      ALIM = .05
000561      WRITE(6,200)
000562  200 FORMAT('THE COMPUTATION SEEMS TO BE OSCILLATING. BECAUSE OF THIS
000563      1. ALIM HAS BEEN SET TO .05 AND THE COMPUTATION RESUMED' /)
000564  149 OLDPOI = PTEGY
000565  100 FLAST = ENERGY
000566      IF(.NOT.NIX)GO TO 103
000567      IF(TIME.LT.UNNIX)GO TO 103
000568      NIX=.FALSE.
000569      DO 101 K=1,MAXNIX
000570      M = INIX(K)
000571      INCV(M)=0
000572  101 CONTINUE
000573      GO TO 103
000574  102 ORICEI = PTEGY
000575      FLAST = FENERGY
000576      OLDPOI = PTEGY
000577  103 CONTINUE
000578      TIME=TIME+DELTIM
000579      ISEC = NSEC
000580      CALL ETIMEI(NSEC)
000581      IF(ISEC.GE.5) GO TO 109
000582      ISEC = NSEC - ISEC
000583      IF(LPT) WRITE(6,16) ISEC

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00n584      IF(AHS(TIME)LT.AOS(TCLOW))
00n585      GO TO 110
00n586      105 IF(LDEL) GO TO 104
00n587      LDEL = .TRUE.
00n588      RESET = .TRUE.
00n589      GO TO 50
00n590      104 WRITE(6,12) IWLMIN  CFQDOT
00n591      GO TO 110
00n592      204 WRITE(6,201)
00n593      201 FORMAT('THE OSCILLATION DESCRIBED ABOVE IS INTOLERABLE. CASE IS
00n594      IREGRETFULLY TERMINATED.' /)
00n595      PERTRR = .FALSE.
00n596      GO TO 110
00n597      109 PERTRR = .FALSE.
00n598      LINOUT = .FALSE.
00n599      LAST = .TRUE.
00n600      110 CONTINUE
00n601      IF(PERTRR.OR.LIFOLT.OB= (.NOT.SAVE)) GO TO 111
00n602      WRITE(13) TITLE
00n603      CALL QTRN(3,1,NWD,AD,IVR)
00n604      IVR = IVR
00n605      38 IF(IVR.EG.-1) GO TO 38
00n606      IF(IVR.LT.NWD) GO TO 125
00n607      CALL NTRN(3,9)
00n608      111 CONTINUE
00n609      AVENTA = PTEGY / MAXNEW
00n610      AVENMA = (PTEGY - SUPEN) / NMOV
00n611      CONEGY = PTEGY - ORIGEN
00n612      WRITE(6,10) AVENTA, MAXNEW, AVENMA, NMOV, CONEGY
00n613      WRITE(6,7) NCU
00n614      WRITE(6,5) (N,X(M),Y(M),Z(M),PCT(M),IMOV(M),KIND(M),M=1,MAXNEW)
00n615      IF(PERTRR.OR.LINOUT) GO TO 112
00n616      IF(PLOT) CALL GPLCT(MAXNEW)
00n617      GO TO 120
00n618      112 CONTINUE
00n619      ICOS = 0
00n620      LOSC = .FALSE.
00n621      IF(.NOT.LINOUT) GO TO 113
00n622      IF(ACOUNT.EG.1) GO TO 107
00n623      DO 114 I=1,MAXNEW
00n624      IMOV(I) = IMOV(1)
00n625      IF(IMOV(I).NE.1) GO TO 106
00n626      IMOV(I) = 0
00n627      GO TO 114
00n628      106 IMOV(I) = 1
00n629      114 CONTINUE
00n630      ACOUNT = 1
00n631      TIME = 0.0
00n632      WRITE(6,9)

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00n633      GO TO 50
00n634      107 \COUNT = 0
00n635      TIME = 0.0
00n636      LINCUT = .FALSE.
00n637      NC 108 I=1,MAXNEW
00n638      IVOV(I) = JNOV(I)
00n639      108 CONTINUE
00n640      WRITE(6,9)
00n641      GO TO 50
00n642      113 IF(.NOT.PERTRB) GO TO 120
00n643      CALL DISTRB
00n644      TSTOP=TSTOP+PERTIM
00n645      PERTRB=.FALSE.
00n646      WRITE(6,9)
00n647      GO TO 50
00n648
00n649      C  \CITE--THE CRYSTAL HAS BEEN RELAXED BEFORE VACANCIES OR INTERSTITIALS
00n650      C  ARE INTRODUCED IF LAX = .TRUE.
00n651      C
00n652      124 WRITE(6,129) IRI, IVP
00n653      GO TO 120
00n654      125 WRITE(6,129) IWIG, IVR
00n655      GO TO 120
00n656      129 FORMAT('ONTRAN DOES NOT LIKE YOU! DIFFICULTIES ENCOUNTERED ', 1A6
00n657      1, 1A1, ' TAPE. IVR = ', 1I6)
00n658      116 WRITE(6,11) DELMAX, EDEL
00n659      GO TO 120
00n660      117 CALL NTRAN(4,8,1)
00n661      120 IF(.NOT.LAST) GO TO 20
00n662      122 IF(SAVE) CALL NTRAN(3,11)
00n663      IF(REPEAT) CALL NTRAN(4,11)
00n664      IF(.NOT.PLOT) GO TO 123
00n665      CALL CPLOT(0.0, -2.0, -3)
00n666      CALL CPLOT(0.0, 0.0, 999)
00n667      123 CONTINUE
00n668      CALL EXIT
00n669      END

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000001      SUBROUTINE CUBE(I2, J2, MSTART)
000002      INCLUDE KST
000003      IF(LRCC) GO TO 1000
000004      IF(NCUB.LEQ.1.OR.NCUB.EQ.100) GO TO 100
000005      IF(NCUB.LEQ.2.OR.NCUB.EQ.110) GO TO 110
000006      IF(NCUB.LEQ.3.OR.NCUB.EQ.111) GO TO 111
000007      IF(NCUB.LEQ.4.OR.NCUB.EQ.112) GO TO 112
000008  C
000009  C      FCC (100) CONFIGURATION
000010  C
000011      100 I1=1
000012      N = MSTART
000013      IF(MOD(I2,2).EQ.0) I2 = I2 + 1
000014      IF(MOD(J2,2).EQ.0) J2 = J2 + 1
000015      DO 1 K=1,K2
000016      DO 2 J=1,J2
000017      DO 3 I=I1,I2
000018      N=N+1
000019      X(N)=I
000020      Y(N)=J
000021      Z(N)=K
000022      3 CONTINUE
000023      IF(I1.EQ.2) I = 0
000024      2 I1=I1+1
000025      1 CONTINUE
000026      XCON = 1.
000027      YCON = 1.
000028      ZCON = 1.
000029      GO TO 2000
000030  C
000031  C      FCC H10 CONFIGURATION
000032  C
000033      110 N = MSTART
000034      S2=SQRT(2.)
000035      U=1.
000036      I1=1
000037      DO 4 K=1,K2
000038      DO 5 J=1,J2
000039      DO 5 I=I1,I2
000040      N=N+1
000041      X(N)=I
000042      Y(N)=U+(J-1)*S2
000043      5 Z(N)=1.+(K-1)*S2/2.
000044      IF(I1.EQ.2) GO TO 6

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```

000045      I1=I1+1
000046      U=1.+S2/2.
000047      GO TO 4
000048  6 I1=1
000049      U=1.
000050  4 CONTINUE
000051      XCON = 1.
000052      YCON = S2
000053      ZCON = S2 / 2.
000054      GO TO 2000
000055
000056  C      FCC (111) CONFIGURATION
000057  C
000058  111 N = MSTART
000059      S2=SQRT(2.)
000060      S22=S2/2.
000061      S62 = SQRT(6.0) / 2.0
000062      S23 = S62 / 3.0
000063      J1=1
000064      I1=1
000065      U=1.
000066      S=1.
000067      CONZ = SQRT(12.0) / 3.0
000068      DO 7 K=1,K2
000069      DO 8 J=1,J2
000070      DO 9 I=1,I2
000071      N=N+1
000072      X(N) = U+(I-1)*S2
000073      Y(N) = S + (J-1) * S62
000074  9 Z(N) = 1. +(K-1)*CONZ
000075      IF (I1.EQ.2)GO TO 10
000076      I1=I1+1
000077      U=1.+S22
000078      GO TO 8
000079  10 I1=1
000080  8 CONTINUE
000081      GO TO(11,12,13), J1
000082  11 S=1.+S23
000083      J1=2
000084      U=1.+S22
000085      GO TO 7
000086  12 S=1.+2.*S23
000087      J1=3
000088      U=1.
000089      GO TO 7
000090  13 S=1.
000091      J1=1
000092      U=1.
000093  7 CONTINUE

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```

00n094      XCON = S2
00n095      YCON = S62
00n096      ZCON = CONZ
00n097      6C TO 2000
00n098
00n099      C
00n100      C   FCC (112) CONFIGURATION
00n101      C
00n102      112 I1 = 1
00n103          M = MSTART
00n104          DELX = SQRT(2.)
00n105          DELX2 = CELX / 2.
00n106          DELY = 2. * SQRT(3.)
00n107          DELY3 = DELY / 3.
00n108          DELY23 = DELY3 * 2.
00n109          DELZ = 2. / SQRT(6.)
00n110          A = 0.
00n111          B = 0.
00n112          DO 20 K=1,K2
00n113          DO 21 J=1,J2
00n114          CC 21 I=1,I2
00n115          M = M + 1
00n116          X(M) = (I-1) * CELX + A + 1.
00n117          Y(M) = (J-1) * DELY + B + 1.
00n118          Z(M) = (K-1) * DELZ + 1.
00n119          I1 = I1 + 1
00n120          A = 0.0
00n121          IF(MOD(I1,2).EQ.0) A = DELX2
00n122          IF(I1.GT.6) 60 TO 22
00n123          IF(I1.EQ.1.OR.I1.EQ.4) 60 TO 23
00n124          IF(I1.EQ.2.OR.I1.EQ.5) 60 TO 29
00n125          R = DELY23
00n126          GC TO 20
00n127          23 B = 0.
00n128          GC TO 20
00n129          24 B = DELY3
00n130          60 TO 20
00n131          22 I1 = 1
00n132          A = 0.
00n133          B = 0.
00n134          20 CCNTINUE
00n135          XCON = DELX
00n136          YCON = DELY
00n137          ZCON = CELZ
00n138          60 TO 2000
00n139      C
00n140      1000 IF(NCUB.EQ.1.OR.NCUB.EQ.100) 60 TO 1100
00n141          IF(NCUB.EQ.2.OR.NCUB.EQ.110) GC TO 1110
00n142      C
00n143      C   RCC (100) CONFIGURATION

```

```

00n143      C
00n144      1100 I1=1
00n145          J1=1
00n146          M=MSTART
00n147          IF(MOD(I2,2).EG.0) I2=I2+1
00n148          IF(MOD(J2,2).EG.0) J2=J2+1
00n149          DO 14 K=1,K2
00n150          DO 15 J=J1,J2,2
00n151          DO 15 I=I1,I2,2
00n152          M=M+1
00n153          X(M)=I
00n154          Y(M)=J
00n155      15 Z(M)=K
00n156          I1=I1+1
00n157          J1=J1+1
00n158          IF(I1.LE.2) GO TO 14
00n159          I1=1
00n160          J1=1
00n161      14 CONTINUE
00n162          XCON = 1.
00n163          YCON = 1.
00n164          ZCON = 1.
00n165          GO TO 2000
00n166      C
00n167      C      HCC (110) CONFIGURATION
00n168      C
00n169      1110 I1=1
00n170          M=MSTART
00n171          IF(MOD(I2,2).EG.0) I2=I2+1
00n172          IF(MOD(J2,2).EG.0) J2=J2+1
00n173          S8=SQRT(R,0) / 2.
00n174          DO 16 K=1,K2
00n175          DO 17 J=J1,J2
00n176          DO 18 I=I1,I2,2
00n177          M=M+1
00n178          X(M)=I
00n179          Y(M)=1.+(J-1)*S8
00n180          Z(M)=1.+(K-1)*S8
00n181      18 CONTINUE
00n182          IF(I1.EG.2) I1=0
00n183      17 I1=I1+1
00n184      16 CONTINUE
00n185          XCON = 1.
00n186          YCON = S8
00n187          ZCON = S8
00n188      C
00n189      C      RETURNING ROUTINE AND BOOKKEEPING (COMMON TO ALL CURES)
00n190      C
00n191      2000 CONTINUE

```

```

00n192      IF (VSTART) , 02001
00n193      AK2 = K2
00n194      G = G * XCON
00n195      XMXX = A12 * YCON
00n196      YMYX = AJ2 * YCON
00n197      ZMXZ = AK2 * ZCON
00n198      GT = (RFEFE(3) + .01) / HLC
00n199      AIC = XMXX - GT
00n200      AJC = YMYX - GT
00n201      AKC = ZMXZ - GT
00n202      AI2 = XMXX
00n203      AJ2 = YMYX
00n204      IF (NCUR.EG.1) NCUR = 100
00n205      IF (NCUR.EG.2) NCUR = 110
00n206      IF (NCUR.EG.3) NCUR = 111
00n207      IF (NCUR.EG.4) NCUR = 112
00n208      2001 MAX = N
00n209      RETURN
00n210      END

```

4. ELT ROTATE,1.690504, 20106

```

00n001      SUBROUTINE ROTATE
00n002      C THIS SUBROUTINE WILL GENERATE A GRAIN BOUNDARY IN THE PLANE THE
00n003      C ROTATION IS ABOUT THE POINT X=6,Y=1: ATOMS WITH X<6 ARE NOT MOVED
00n004      INCLUDE KST
00n005      DIST(XX,YY)=SQRT(XX*XX+YY*YY)
00n006      K = 0
00n007      ALPHA = DEG * .0174532925
00n008      H = G / XCON
00n009      AI2 = AI2 / XCON
00n010      AJ2 = AJ2 / YCON
00n011      MAX1 = MAX + 1
00n012      AI2G = AI2 - H + 2.
00n013      SINALP = SIN(ALPHA)
00n014      COSALP = COS(ALPHA)
00n015      A = AI2G * COSALP
00n016      XCOR = AI2 - A * COSALP
00n017      YCOR = 1. - A * SINALP
00n018      I2NEW = A + SINALP * AJ2 + 1.
00n019      J2NEW = COSALP * AJ2 + SINALP * AI2G + 2.
00n020      C
00n021      DO 21 M=1,MAX
00n022      IF(X(M).LT.(G-REJ)) GO TO 21
00n023      K = K + 1
00n024      N(K) = M
00n025      X1(K) = X(M)
00n026      Y1(K) = Y(M)
00n027      Z1(K) = Z(M)
00n028      21 CONTINUE
00n029      C
00n030      G = H
00n031      CALL CLBE(I2NEW, J2NEW, MAX)
00n032      C
00n033      DO 60 M=MAX1, AX
00n034      X(M) = X(M) - 1.
00n035      Y(M) = Y(M) - 1.
00n036      CC = DIST(X(M), Y(M))
00n037      THETA = ACOS(X(M) / CC)
00n038      RHO = THETA + ALPHA
00n039      X(M) = CC * COS(RHO) + XCOR
00n040      Y(M) = CC * SIN(RHO) + YCOR
00n041      IF(Y(M).LT.1. OR X(M).LT.G OR X(M).GT.AI2 OR Y(M).GT.AJ2) GO TO 147
00n042      IF(X(M).GT.(G+REJ)) GO TO 60
00n043      C
00n044      DO 31 M=1,K

```

```

00n045      IF(Y1(M1)+REJ.LT.Y(M).OR.Y1(M1)-REJ.GT.Y(M).OR.Z1(M1)+REJ.LT.Z(M)
00n046      .OR.Z1(M1)-REJ.GT.Z(M)) GO TO 31
00n047      R = SQRT((X(M)-X1(M1))**2 + (Y(M)-Y1(M1))**2 + (Z(M)-Z1(M1))**2)
00n048      IF(R.GT.REJ) GO TO 31
00n049      30 X(M)=-1.0
00n050      31 CONTINUE
00n051      C
00n052      GO TO 60
00n053      147 X(M) = -1.
00n054      60 CONTINUE
00n055      C
00n056      RETURN
00n057      END

```

4 ELT DISLOC,1,690508, 20114

```

000001      SUBROUTINE DISLOC
000002      INCLUDE KST
000003      LOGICAL LEVEN, Z8EPV
000004      PI = 3.1415927
000005      CAD1 = -E1 * PI / 2.
000006      IM = 4
000007      IF(LPART) IM = 0
000008      DELZ = ZCON
000009      LPRCV = .TRUE.
000010      RUMR = -1.0
000011      IF(YDISP2.GT.YDISPL) LSTACK = .FALSE.
000012      ZCON = 1.
000013      DISCOR = XCON / 2.
000014      XPD = XCON + .9
000015      YPD = YCON + .6
000016      RVECT = 2.
000017      IF(ACUR.EQ.111.OR.ACUR.EQ.112) BVECT = SQRT(2.)
000018      XDIS = XDISPL * XCON + 1.
000019      YDIS = YDISPL * YCON + 1.
000020      XDISPL = XDIS
000021      YDISPL = YDIS
000022      DX2 = XCON / 2. + 0.1
000023      LEVEN = .FALSE.
000024      IF(.NOT.LRCC) GO TO 7
000025      DO 2 I=1,MAX
000026      I = I + 1
000027      IF(X(I).LT.X(1)) GO TO 3
000028      2 CONTINUE
000029      3 I = I - 1
000030      XOUT = X(I) + 0.1
000031      I = I - 1
000032      XFIX = X(I) + 0.1
000033      NMOV = 0
000034      DO 6 I=1,MAX
000035      IF(X(I).LT.XBD.OR.Y(I).LT.YBD.OR.X(I).GT.AIC.OR.Y(I).GT.AJC)GO TO 4
000036      IVCV(I) = IM
000037      NMOV = NMOV + 1
000038      GO TO 5
000039      4 IVCV(I) = 1
000040      5 IF(X(I).LT.XFIX.OR.Y(I).GT.YDISPL) GO TO 6
000041      IF(X(I).GT.XOUT) X(I) = -1.0
000042      IF(IVCV(I).EQ.IM) NMOV = NMOV - I
000043      IVCV(I) = 1
000044

```

```

00n045      6 CONTINUE
00n046      GO TO 11
00n047      CAD1 = 0.0
00n048      IF(.NOT.LBDRY) GO TO 10
00n049      NMOV = 0
00n050      DO 4 I=1,MAX
00n051      IF(X(I).LT.XBD.OR.Y(I).LT.YBD.OR.X(I).GT.AIC.OR.Y(I).GT.AJC)GOTO 8
00n052      INCV(I) = IM
00n053      NMOV = NMOV + 1
00n054      GO TO 9
00n055      8 INOV(I) = 1
00n056      9 CONTINUE
00n057      LBDRY = .FALSE.
00n058      10 DO 12 I=1,MAX
00n059      XDX = X(I) - XDIS
00n060      PCT(I) = XDX
00n061      IF(ABS(Z(I)-ZCORD).LT..2) GO TO 17
00n062      ZCORD = ZCORD + CELZ
00n063      IF(LEVEN) GO TO 15
00n064      XDIS = XDIS + DISCOR
00n065      LEVEN = .TRUE.
00n066      GO TO 17
00n067      15 XDIS = XDIS - DISCOR
00n068      LEVEN = .FALSE.
00n069      17 CONTINUE
00n070      IF(XDX.GT.-DX2.AND.XDX.LT..01.AND.Y(I).LT.YDIS) X(I) = -1.0
00n071      IF(XDX.GE..01.AND.XDX.LT.DX2.AND.Y(I).LT.YDIS) X(I) = X(I)-DX2-.01
00n072      IF(INOV(I).EQ.IM.AND.X(I).LT.0.0) NMOV = NMOV - 1
00n073      12 CONTINUE
00n074      11 IF(ISO) 60 TO 50
00n075      ALFA = C11 + C12 + 2.*C44
00n076      BETA = C11 - C12
00n077      GAMA = C11 * C44
00n078      DLTA = C12 - C11 + 2.*C44
00n079      EPSL = C11 + C12
00n080      RHO = C11**2 - C12**2
00n081      AC = 0.5 * SQRT(ALFA * BETA / GAMA)
00n082      RC = 0.5 * SQRT(DLTA * EPSL / GAMA)
00n083      CO = SQRT(RHO * ALFA * DLTA) / (2. * GAMA)
00n084      DO = EPSL * DLTA / (2. * GAMA) - 1.
00n085      EC = 0.5 * SQRT(RHO / (ALFA * DLTA))
00n086      FC = 0.5 * SQRT(C44 * BETA / (C11 * ALFA))
00n087      GC = SQRT(C44 * EPSL / (C11 * DLTA))
00n088      DO 20 I=1,MAX
00n089      IF(X(I).LT.0.0) GO TO 20
00n090      XD = X(I) - XDISPL
00n091      IF(.NOT.LBCC) XD = PCT(I)
00n092      YD = Y(I) - YDISPL
00n093      CAD = CAD1

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```

00n094      IF(XD.GT.0..AND.YD.GT.0.) CAD = CAD / (-3.)
00n095      LX = -RVECT / 2. * (ATAN(2.*XD*YD*AD / (XD**2-YD**2)) + CAD + ED *
00n096      1 LOG((XD**2 + YD**2 + 2.*XD*YD*BD) / (XD**2+YD**2-2.*XD*YD*BD)))
00n097      LY = -RVECT / 2. * (ED*LOG((XD**2+YD**2)**2-4.*XD**2*YD**2*BD**2)
00n098      1 - GD) + ATAN(YD**2*CD) / (XD**2-YD**2 * CD))
00n099      X(I) = X(I) + LX
00n100      Y(I) = Y(I) + LY
00n101      20 CONTINUE
00n102      RETURN
00n103      50 DO 60 I=1,MAX
00n104      IF(X(I).LT.0.0) GO TO 60
00n105      XD = X(I) - XDISPL
00n106      IF(.NOT.LBCC) XD = PCT(I)
00n107      YD = Y(I) - YDISPL
00n108      CAD = CAD1
00n109      IF(XD.GT.0..AND.YD.GT.0.) CAD = CAD / (-3.)
00n110      51 LX = RVECT / (2.*PI) * (ATAN(YD/XD) + XD*YD / (2.*(1.-PR) * (XD**2
00n111      1 + YD**2)) + CAD)
00n112      LY = -RVECT / (2.*PI) * ((1.-2.*PR)/(4.*(1.-PR))*LOG(XD**2+YD**2)
00n113      1 + (XD**2-YD**2) / (4.*(1.-PR)*(XD**2+YD**2)))
00n114      X(I) = X(I) + LX
00n115      Y(I) = Y(I) + LY
00n116      60 CONTINUE
00n117      IF(DUMR.GT.0.0) YDISPL = DUMR
00n118      DUMR = YDISPL
00n119      IF(.NOT.LSTACK) RETURN
00n120      LSTACK = .FALSE.
00n121      YDISPL = YDISP2
00n122      GO TO 1
00n123      END

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ELI DISTRB,1,690508, 20121

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00n001      SUBROUTINE DISTRB
00n002      INCLUDE KST
00n003      ALIM = 0.4
00n004      IF(.NOT.VAC)GO TO 10
00n005      DO 2 J=1,NVAC
00n006      M = NVAC(J)
00n007      X(M)=-99.0
00n008      INCV(M)=1
00n009      KING(M)=77
00n010      PCT(M)=0.0
00n011      2 CONTINUE
00n012      10 IF(.NOT.LMOVE) GO TO 11
00n013      DO 20 K=1,MMOVE
00n014      N = MOVE(K)
00n015      X(N) = AMOVE(K,1)
00n016      Y(N) = AMOVE(K,2)
00n017      Z(N) = AMOVE(K,3)
00n018      20 CONTINUE
00n019      11 IF(.NOT.LADD) GO TO 15
00n020      IF(LINT) GO TO 13
00n021      INT1 = MAXNEW + 1
00n022      LINT = .TRUE.
00n023      13 DO 5 L=1,ADATM
00n024      M=MAXNEW+1
00n025      MAXNEW=M
00n026      12 X(M)=ADATM(L,1)
00n027      Y(M)=ADATM(L,2)
00n028      Z(M)=ADATM(L,3)
00n029      KING(M) = ADATM(L,4) + .001
00n030      INCV(M)=0
00n031      TXVEL(M)=0.0
00n032      TYVEL(M)=0.0
00n033      TZVEL(M)=0.0
00n034      PCT(M)=0.0
00n035      5 CONTINUE
00n036      RESET=.TRUE.
00n037      ADD = .TRUE.
00n038      15 IF(.NOT.NIX)GO TO 30
00n039      UNNIX=TIME+TIMNIX
00n040      DO 34 L=1,MAXNIX
00n041      DO 37 M=1,MAXNEW
00n042      IF(.EG.NIXX(L))INCV(M)=2
00n043      IF(.EG.NIXY(L))INCV(M)=3
00n044      IF(.EG.NIXZ(L))INCV(M)=4

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000045	IF(M.NE.INIX(L))GO TO 37
000046	INOV(M)=1
000047	37 CONTINUE
000048	38 CONTINUE
000049	30 RETI PL
000050	END

W. ELT GPLOT ,690508, 20130

```

00n001      SUBROUTINE GPLOT(MA)
00n002      INCLUDE KST
00n003      XMAX = A12 / 2. + 1.
00n004      48 YMAX = A22 / 2. + 1.
00n005      IF(PLTXZ) YMAX = ZMXZ / 2. + 1.
00n006      W = XMAX
00n007      H = YMAX
00n008      IF(PLTLU) GO TO 49
00n009      NREP = 2
00n010      IF(NCUR.EQ.111 OR NCUR.EQ.3) NREP = 3
00n011      J1 = NREP + 1
00n012      PT1 = 1.3
00n013      PT2 = 1.3 + ZCON
00n014      PT3 = 1.3 + ZCON * (NREP-1)
00n015      IF(K2.GT.NREP) J1 = K2 + 1
00n016      NPL = 1
00n017      IF(.NOT.PLTXZ) GO TO 51
00n018      J1 = (A22 + .1) / YCON + 1
00n019      NREP = 0
00n020      NPL = 1
00n021      GO TO 51
00n022      49 J1 = NPL + 1
00n023      IF(IPU.LT.NPL) J1 = NPL + 1
00n024      NREP = 0
00n025      51 GO TO J=NPL,J1
00n026      IF (J.EQ.J1.AND.J1.GT.NREP+1) GO TO 40
00n027      XTP = .5
00n028      YTP = YMAX + 3.
00n029      CALL SYMRCL(XTP, YTP, .119, TITLE(1), 0.0, 80)
00n030      YTP = YTP - .4
00n031      CALL SYMRCL(XTP, YTP, .119, TITLE(15), 0.0, 80)
00n032      YTP = YMAX + 2.
00n033      IF(LRCC) GO TO 300
00n034      IF(NCUR.EQ.100 OR NCUR.EQ.1) GO TO 101
00n035      IF(NCUR.EQ.110 OR NCUR.EQ.2) GO TO 102
00n036      IF(NCUR.EQ.112 OR NCUR.EQ.4) GO TO 100
00n037      CALL SYMRCL(XTP, YTP, .175, 56, 'THIS PLOT IS OF AN FCC LATTICE VIEWED
00n038      IN THE (111) PLANE , 0.0, 56)
00n039      GO TO 103
00n040      102 CALL SYMRCL(XTP, YTP, .175, 56, 'THIS PLOT IS OF AN FCC LATTICE VIEWED
00n041      IN THE (110) PLANE , 0.0, 56)
00n042      GO TO 103
00n043      101 CALL SYMRCL(XTP, YTP, .175, 56, 'THIS PLOT IS OF AN FCC LATTICE VIEWED
00n044      IN THE (100) PLANE , 0.0, 56)

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000045      GO TO 103
000046 100 CALL SYMPCCL(XTP, YTP, .175, 56) THIS PLOT IS OF AN FCC LATTICE VIEWED
000047    IN THE (112) PLANE , 0.0, 56)
000048      GO TO 103
000049 300 IF(NCLR.EQ.110.CR.NCLR.EQ.2) GO TO 301
000050    CALL SYMPCCL(XTP, YTP, .175, 56) THIS PLOT IS OF A FCC LATTICE VIEWED
000051    IN THE (100) PLANE , 0.0, 56)
000052      GO TO 103
000053 301 CALL SYMPCCL(XTP, YTP, .175, 56) THIS PLOT IS OF A FCC LATTICE VIEWED
000054    IN THE (110) PLANE , 0.0, 56)
000055 103 YIP = YIP - 0.3
000056    IF(.NOT.PLTXZ) GO TO 99
000057    CALL SYMPCCL(XTP, YTP, .161, 56) THE PLANES ARE FOR [X,Z] RATHER THAN
000058    [X,Y] ORIENTATION, 0.0, 54)
000059    YTP = YTP - 0.3
000060 99 IF(.NOT.LCISL) GO TO 303
000061    IF(YDISP2.LT.1.0) GO TO 94
000062    CALL SYMPCCL(XTP, YTP, .154, 56) STACKED DISLOCATION AT X =      , Y1
000063    1 =      , Y2 = , 0.0, 52)
000064    CALL NUMBER(4.66, YTP, .154, XDISPL, 0.0, 1)
000065    CALL NUMBER(6.67, YTP, .154, YDISPL, 0.0, 1)
000066    CALL NUMBER(8.17, YTP, .154, YDISP2, 0.0, 1)
000067    YTP = YIP - 0.3
000068      GO TO 303
000069 94 CONTINUE
000070    CALL SYMPCCL(XTP, YTP, .154, 56) DISLOCATION AT X =      , Y = , 0.0,
000071    1 29)
000072    CALL NUMBER(3.45, YTP, .154, XDISPL, 0.0, 1)
000073    CALL NUMBER(5.15, YTP, .154, YDISPL, 0.0, 1)
000074    YTP = YIP - 0.3
000075 303 IF(.NOT.GRAIN) GO TO 104
000076    CALL SYMPCCL(XTP, YTP, .154, 56) GRAIN BOUNDARY AT X =      IS FOR A RO
000077    TATION OF      DEGREES , 0.0, 59)
000078    CALL NUMBER( 7.55, YTP, .154, DFG, 0.0, 2)
000079    CALL NUMBER(3.7, YTP, .154, G, 0.0, 0)
000080    YTP = YIP - 0.3
000081 104 IF(.NOT.VAC) GO TO 105
000082    CALL SYMPCCL(XTP, YTP, .154, 56) THERE ARE      VACANCIES IN THIS LAT
000083    TICE , 0.0, 39)
000084    FPN = MVAC
000085    CALL NUMBER(1.98, YTP, .154, FPN, 0.0, -1)
000086    YTP = YIP - 0.3
000087 105 IF(.NOT.ACI) GO TO 106
000088    CALL SYMPCCL(XTP, YTP, .154, 43) THERE ARE      INTERSTITIALS IN THIS
000089    LATTICE , 0.0, 43)
000090    FPN = MACATM
000091    CALL NUMBER(1.98, YTP, .154, FPN, 0.0, -1)
000092    YTP = YIP - 0.3
000093 106 IF(.EQ.1) GO TO 151

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000094      IF(.NOT.PLTXYZ) GO TO 97
000095      CALL SYMROL(XTP, YTP, .154, 'THIS PLANE IS: Y =', 0.0, 19)
000096      GO TO 98
000097      97 CALL SYMROL(XTP, YTP, .154, 'THIS PLANE IS: Z =', 0.0, 19)
000098      98 FPN = 0
000099      CALL NUMBER(3.5, YTP, .154, FPN, 0.0, -1)
000100      151 XTP = 2.
000101          YTP = -.52
000102      CALL SYMROL(XTP, YTP, .189, 29 HUNITS = HALF LATTICE CONSTANT, 0.0, 29)
000103          YTP = YTP - .03
000104      CALL SYMROL(XTP, YTP, .14, 43 H(1 HALF LATTICE CONSTANT = AN
000105      1GSTRONS), 0.0, 43)
000106      CALL NUMBER(5.75, YTP, .14, HLC, 0.0, 3)
000107          XPT = 0.75
000108      DO 107 K=1,50
000109          CALL CPLLOT(XPT, 0.0, 3)
000110          IF(MOD(K,2).EQ.0) GO TO 206
000111          CALL CPLLOT(XPT, 0.2, 2)
000112          CALL CPLLOT(XPT, 0.0, 2)
000113          ANUM = K
000114          XKY = XPT - .14
000115          IF(K.LT.10) XKY = XPT - .07
000116          CALL NUMBER(XKY, -.21, .14, ANUM, 0.0, -1)
000117      GO TO 207
000118      206 CALL CPLLOT(XPT, .1, 2)
000119          CALL CPLLOT(XPT, 0.0, 2)
000120      207 XPT = XPT + 0.5
000121          IF(XPT.GT.XMAX+.25) GO TO 108
000122      107 CONTINUE
000123      108 CALL CPLLOT(XMAX, 0.0, 3)
000124          CALL CPLLOT(0.0, 0.0, 2)
000125          CALL CPLLOT(0.0, YMAX, 2)
000126          CALL CPLLOT(XMAX, YMAX, 2)
000127          CALL CPLLOT(XMAX, 0.0, 2)
000128          XPT = 0.75
000129          HW5 = H - 0.1
000130          HW1 = H - 0.2
000131      DO 113 K=1,50
000132          CALL CPLLOT(XPT, H, 3)
000133          IF(MOD(K,2).EQ.0) GO TO 213
000134          CALL CPLLOT(XPT, HW1, 2)
000135          CALL CPLLOT(XPT, H, 2)
000136      GO TO 712
000137      213 CALL CPLLOT(XPT, HW5, 2)
000138          CALL CPLLOT(XPT, H, 2)
000139      212 XPT = XPT + 0.5
000140          IF(XPT.GT.W+.25) GO TO 114
000141      113 CONTINUE
000142      114 W1 = W - 0.2

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000143      WWS = W - 0.1
000144      YPT = 0.75
000145      DO 115 K=1,50
000146      CALL CPLOT( W , YPT, 3)
000147      IF(WDD(K,2).EQ.0) GO TO 215
000148      CALL CPLOT(WM1, YPT, 2)
000149      CALL CPLOT(W, YPT, 2)
000150      GO TO 214
000151 215 CALL CPLOT(WWS, YPT, 2)
000152      CALL CPLOT(W, YPT, 2)
000153 214 YPT = YPT + 0.5
000154      IF(YPT.GT.H-.25) GO TO 116
000155 115 CONTINUE
000156 116 YPT = 0.75
000157      DO 109 K=1,50
000158      CALL CHLOT(0.0, YPT, 3)
000159      IF(WDD(K,2).EQ.1) GO TO 208
000160      CALL COLOT(0.2, YPT, 2)
000161      CALL COLOT(0.0, YPT, 2)
000162      ANUM = K
000163      XKT = -.4
000164      IF(K.LT.10) XKT = -.26
000165      CALL NUMRED(XKT, YPT-.07, .14, ANUM, 0.0, -1)
000166      GO TO 209
000167 208 CALL CPLOT(0.1, YPT, 2)
000168      CALL OPLOT(0.0, YPT, 2)
000169 209 YPT = YPT + 0.5
000170      IF(YPT.GT.YMAX-.25) GO TO 110
000171 109 CONTINUE
000172 110 XTP = -.05
000173      YTP = 2.
000174      CALL SYMBOL(XTP,YTP,.154,29HUNITS - HALF LATTICE CONSTANT,90.0,29)
000175      XTP = -.55
000176      CALL SYMBOL(XTP, YTP, .14 , 43H(1 HALF LATTICE CONSTANT =      AN
000177      16STROMSI , 90.0, 43)
000178      CALL NUMBER(XTP, 5.75, .14, HLC, 90.0, 3)
000179      CCNZ = ZCCN
000180      IF(PLTXZ) CCNZ = YCCN
000181      ZMAX = 0.499 + CCNZ * J
000182      ZMIN = 0.5 + CCNZ * (J-1)
000183 C
000184      DO 1 I=1,NA
000185      ZP = Z(1)
000186      IF(PLTXZ) ZP = Y(1)
000187      IF((ZP.GT.ZMAX.OR.ZP.LT.ZMIN).AND.J.NE.1) GO TO 1
000188      K1I = K1ND(1)
000189      IF(K1I.GT.5) GO TO 1
000190      RAT = 0.0
000191      IF(1.GE.MAX1) RAT = DEF

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00n192      XF = X(1) / 2. + .25
00n193      YP = Y(1) / 2. + .25
00n194      IF(PLTX2) YP = Z(1) / 2. + .25
00n195      XP1 = XF - .1
00n196      YP1 = YP - .15
00n197      CALL CPLOT(XP, YP, 3)
00n198      IF(J.EQ.01) GO TO 199
00n199      IF(IMCV(I).EQ.1.AND.KII.EQ.1) GO TO 30
00n200      GO TO (31,32,33,34,35), KII
00n201      31 CALL SYMRCL(XP, YP, 0.637, 1, RAT, -1)
00n202      GO TO 20
00n203      32 CALL SYMRCL(XP, YP, 0.49, 2, 0.0, -1)
00n204      GO TO 20
00n205      33 CALL SYMRCL(XP, YP, 0.637, 5, 0.0, -1)
00n206      GO TO 20
00n207      34 CALL SYMRCL(XP, YP, 0.637, 10, 0.0, -1)
00n208      GO TO 20
00n209      35 CALL SYMRCL(XP, YP, 0.637, 30, 0.0, -1)
00n210      GO TO 20
00n211      30 CALL SYMRCL(XP, YP, 0.637, 0, RAT, -1)
00n212      GO TO 20
00n213      159 IF(Z(I).GT.PT1) GO TO 8
00n214      IF(IMCV(I).EQ.1.AND.KII.EQ.1) GO TO 7
00n215      GO TO (2,3,4,5,6), KII
00n216      2 CALL SYMRCL(XP, YP, 0.49, 1, RAT, -1)
00n217      GO TO 20
00n218      3 CALL SYMRCL(XP, YP, 0.21, 2, 0.0, -1)
00n219      GO TO 1
00n220      4 CALL SYMRCL(XP, YP, 0.49, 5, 0.0, -1)
00n221      GO TO 20
00n222      5 CALL SYMRCL(XP, YP, 0.49, 10, 0.0, -1)
00n223      GO TO 20
00n224      6 CALL SYMRCL(XP, YP, 0.49, 30, 0.0, -1)
00n225      GO TO 20
00n226      7 CALL SYMRCL(XP, YP, 0.63, 0, RAT, -1)
00n227      GO TO 20
00n228      8 IF(Z(I).GT.PT2) GO TO 15
00n229      IF(IMCV(I).EQ.1.AND.KII.EQ.1) GO TO 14
00n230      GO TO (9,10,11,12,13), KII
00n231      9 CALL SYMRCL(XP, YP, 0.35, 1, RAT, -1)
00n232      GO TO 20
00n233      10 CALL SYMRCL(XP, YP, 0.14, 2, 0.0, -1)
00n234      GO TO 1
00n235      11 CALL SYMRCL(XP, YP, 0.35, 5, 0.0, -1)
00n236      GO TO 20
00n237      12 CALL SYMRCL(XP, YP, 0.35, 10, 0.0, -1)
00n238      GO TO 20
00n239      13 CALL SYMRCL(XP, YP, 0.35, 30, 0.0, -1)
00n240      GO TO 20

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00n241      14 CALL SYMROL(XP, YP, 0.49, 0, RAT, -1)
00n242      GC TO 20
00n243      15 IF(Z(I).GT.PT3) GC IC 1
00n244      IF(IMCV(I).EQ.1.AND.KII.EQ.1) GO TO 22
00n245      GC TO (16,17,18,19,21), KII
00n246      16 CALL SYMROL(XP, YP, 0.42, 1, RAT, -1)
00n247      GC TO 20
00n248      17 CALL SYMROL(XP, YP, .182, 2, 0.0, -1)
00n249      GC TO 1
00n250      18 CALL SYMROL(XP, YP, 0.42, 5, 0.0, -1)
00n251      GC TO 20
00n252      19 CALL SYMROL(XP, YP, 0.42, 10, 0.0, -1)
00n253      GC TO 20
00n254      21 CALL SYMROL(XP, YP, 0.42, 30, 0.0, -1)
00n255      GC TO 20
00n256      22 CALL SYMROL(XP, YP, 0.54, 0, RAT, -1)
00n257      20 FPN = 1
00n258      CALL CPLOT(XP1, YP1, 3)
00n259      CALL NUMBER(XP1, YP1, 0.091, FPN, 0.0, -1)
00n260      CALL CPLOT(XP1, YP1, 3)
00n261      CALL NUMBER(XP1, YP1, 0.091, FPN, 0.0, -1)
00n262      1 CONTINUE
00n263      C
00n264      CALL CPLOT(XMAX + 5., 0.0, -3)
00n265      40 CONTINUE
00n266      C
00n267      IF(.NOT.PLTIXZ) RETURN
00n268      PLTIXZ = .FALSE.
00n269      PLTLU = .FALSE.
00n270      GC TO 48
00n271      END

```


APPENDIX B

SAMPLE PROBLEM

B
t[illegible]

	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
LMOVE = F,	,	,	,	,	,	,	,
MMOVE =	,	,	,	,	,	,	,
MOVE =	,	,	,	,	,	,	,
AMOVE =	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
NIX = F,	,	,	,	,	,	,	,
MAXNIX =	,	,	,	,	,	,	,
INIX =	,	,	,	,	,	,	,
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NIXX =	,	,	,	,	,	,	,
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NIXY =	,	,	,	,	,	,	,
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	,	,	,	,	,	,	,
NIXZ =	,	,	,	,	,	,	,
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	,	,	,	,	,	,	,
	,	,	,	,	,	,	,
	,	,	,	,	,	,	,
	,	,	,	,	,	,	,
TIMNIX =	.00000000+00,						
LINT = F,	,						
INT1 =	,						
PRTIM =	.10000000+00,						
DELTIM =	.10000000+00,						
ALIM =	.40000000+00,						

TIME	POTENTIAL ENERGY	KINETIC ENERGY	TOTAL ENERGY	MAXIMUM KINETIC ENERGY	SURFACE ENERGY (POT)
.000	-973.684610	2.0536661-18	-973.684610	1.3803598-20 (116)	-398.280730
1.000	-973.684610	1.8483005-17	-973.684610	1.2423239-19 (116)	-398.280730
1.000	-973.684610	2.0536661-18	-973.684610	1.3803598-20 (116)	-398.280730

RUN TERMINATED BECAUSE TOTAL ENERGY CHANGE IS LESS THAN 5.00000-U6. DELPOT = 0.00000

ON THE LAST TIME STEP THE AVERAGE POTENTIAL ENERGY PER ATOM IS: -1.2356404+00, AND THE TOTAL NUMBER OF ATOMS IS: 788

THE AVERAGE POTENTIAL ENERGY PER MOVABLE ATOM IS: -1.3570846+00, AND THE NUMBER OF MOVABLE ATOMS IS: 424

CONFIGURATION ENERGY = -0.0000000

CRYSTAL AFTER RELAXATION (100) ORIENTATION OF (X,Y) PLANES
(MOVABLE ATOMS ARE NOTED BY A TAG OF 0; IMMOVABLE ATOMS BY A TAG OF 1)

ATOM	X	Y	Z	P.ENERGY	TAG	TYPE	ATOM	X	Y	Z	P.ENERGY	TAG	TYPE
1	1.000000	1.000000	1.000000	-.3752646	1	1	2	3.000000	1.000000	1.000000	-.625441	1	1
3	5.000000	1.000000	1.000000	-.6254411	1	1	4	7.000000	1.000000	1.000000	-.625441	1	1
5	2.000000	2.000000	1.000000	-1.0007057	1	1	6	4.000000	2.000000	1.000000	-1.000706	1	1
7	6.000000	2.000000	1.000000	-1.0007057	1	1	8	1.000000	3.000000	1.000000	-.625441	1	1
9	3.000000	3.000000	1.000000	-1.0007057	0	1	10	5.000000	3.000000	1.000000	-1.000706	0	1
11	7.000000	3.000000	1.000000	-1.0007057	0	1	12	2.000000	4.000000	1.000000	-1.000706	1	1
13	4.000000	4.000000	1.000000	-1.0007057	0	1	14	6.000000	4.000000	1.000000	-1.000706	0	1
15	1.000000	5.000000	1.000000	-.6254411	1	1	16	3.000000	5.000000	1.000000	-1.000706	0	1
17	5.000000	5.000000	1.000000	-1.0007057	0	1	18	7.000000	5.000000	1.000000	-1.000706	0	1
19	2.000000	6.000000	1.000000	-1.0007057	1	1	20	4.000000	6.000000	1.000000	-1.000706	0	1
21	6.000000	6.000000	1.000000	-1.0007057	0	1	22	1.000000	7.000000	1.000000	-.625441	1	1
23	3.000000	7.000000	1.000000	-1.0007057	0	1	24	5.000000	7.000000	1.000000	-1.000706	0	1
25	7.000000	7.000000	1.000000	-1.0007057	0	1	26	2.000000	8.000000	1.000000	-1.000706	1	1
27	4.000000	8.000000	1.000000	-1.0007057	0	1	28	6.000000	8.000000	1.000000	-1.000706	0	1
29	1.000000	9.000000	1.000000	-.6254411	1	1	30	3.000000	9.000000	1.000000	-1.000706	0	1
31	5.000000	9.000000	1.000000	-1.0007057	0	1	32	7.000000	9.000000	1.000000	-1.000706	0	1
33	2.000000	10.000000	1.000000	-1.0007057	1	1	34	4.000000	10.000000	1.000000	-1.000706	0	1
35	6.000000	10.000000	1.000000	-1.0007057	0	1	36	1.000000	11.000000	1.000000	-.625441	1	1
37	3.000000	11.000000	1.000000	-1.0007057	0	1	38	5.000000	11.000000	1.000000	-1.000706	0	1
39	7.000000	11.000000	1.000000	-1.0007057	0	1	40	2.000000	12.000000	1.000000	-1.000706	1	1
41	4.000000	12.000000	1.000000	-1.0007057	0	1	42	6.000000	12.000000	1.000000	-1.000706	0	1
43	1.000000	13.000000	1.000000	-.6254411	1	1	44	3.000000	13.000000	1.000000	-1.000706	0	1
45	5.000000	13.000000	1.000000	-1.0007057	0	1	46	7.000000	13.000000	1.000000	-1.000706	0	1
47	2.000000	14.000000	1.000000	-1.0007057	1	1	48	4.000000	14.000000	1.000000	-1.000706	1	1
49	6.000000	14.000000	1.000000	-1.0007057	1	1	50	1.000000	15.000000	1.000000	-.375265	1	1
51	3.000000	15.000000	1.000000	-.6254411	1	1	52	5.000000	15.000000	1.000000	-.625441	1	1
53	7.000000	15.000000	1.000000	-.6254411	1	1	54	2.000000	1.000000	2.000000	-1.000706	1	1
55	4.000000	1.000000	2.000000	-1.0007057	1	1	56	6.000000	1.000000	2.000000	-1.000706	1	1
57	1.000000	2.000000	2.000000	-1.0007057	1	1	58	3.000000	2.000000	2.000000	-1.501059	1	1
59	5.000000	2.000000	2.000000	-1.5010586	1	1	60	7.000000	2.000000	2.000000	-1.501059	1	1
61	2.000000	3.000000	2.000000	-1.5010586	1	1	62	4.000000	3.000000	2.000000	-1.501059	0	1
63	6.000000	3.000000	2.000000	-1.5010586	0	1	64	1.000000	4.000000	2.000000	-1.000706	1	1
65	3.000000	4.000000	2.000000	-1.5010586	0	1	66	5.000000	4.000000	2.000000	-1.501059	0	1
67	7.000000	4.000000	2.000000	-1.5010586	0	1	68	2.000000	5.000000	2.000000	-1.501059	1	1
69	4.000000	5.000000	2.000000	-1.5010586	0	1	70	6.000000	5.000000	2.000000	-1.501059	0	1
71	1.000000	6.000000	2.000000	-1.0007057	1	1	72	3.000000	6.000000	2.000000	-1.501059	0	1
73	5.000000	6.000000	2.000000	-1.5010586	0	1	74	7.000000	6.000000	2.000000	-1.501059	0	1
75	2.000000	7.000000	2.000000	-1.5010586	1	1	76	4.000000	7.000000	2.000000	-1.501059	0	1
77	6.000000	7.000000	2.000000	-1.5010586	0	1	78	1.000000	8.000000	2.000000	-1.000706	1	1
79	3.000000	8.000000	2.000000	-1.5010586	0	1	80	5.000000	8.000000	2.000000	-1.501059	0	1
81	7.000000	8.000000	2.000000	-1.5010586	0	1	82	2.000000	9.000000	2.000000	-1.501059	1	1
83	4.000000	9.000000	2.000000	-1.5010586	0	1	84	6.000000	9.000000	2.000000	-1.501059	0	1

85	1.000000	10.000000	2.000000	-1.0007057	1	1
87	5.000000	10.000000	2.000000	-1.5010586	0	1
89	2.000000	11.000000	2.000000	-1.5010586	1	1
91	6.000000	11.000000	2.000000	-1.5010586	0	1
93	3.000000	12.000000	2.000000	-1.5010586	0	1
95	7.000000	12.000000	2.000000	-1.5010586	0	1
97	4.000000	13.000000	2.000000	-1.5010586	0	1
99	1.000000	14.000000	2.000000	-1.0007057	1	1
101	5.000000	14.000000	2.000000	-1.5010586	1	1
103	2.000000	15.000000	2.000000	-1.0007057	1	1
105	6.000000	15.000000	2.000000	-1.0007057	1	1
107	3.000000	1.000000	3.000000	-1.0007057	1	1
109	7.000000	1.000000	3.000000	-1.0007057	1	1
111	4.000000	2.000000	3.000000	-1.5010586	1	1
113	1.000000	3.000000	3.000000	-1.0007057	1	1
115	5.000000	3.000000	3.000000	-1.5010586	0	1
117	2.000000	4.000000	3.000000	-1.5010586	1	1
119	6.000000	4.000000	3.000000	-1.5010586	0	1
121	3.000000	5.000000	3.000000	-1.5010586	0	1
123	7.000000	5.000000	3.000000	-1.5010586	0	1
125	4.000000	6.000000	3.000000	-1.5010586	0	1
127	1.000000	7.000000	3.000000	-1.0007057	1	1
129	5.000000	7.000000	3.000000	-1.5010586	0	1
131	2.000000	8.000000	3.000000	-1.5010586	1	1
133	6.000000	8.000000	3.000000	-1.5010586	0	1
135	3.000000	9.000000	3.000000	-1.5010586	0	1
137	7.000000	9.000000	3.000000	-1.5010586	0	1
139	4.000000	10.000000	3.000000	-1.5010586	0	1
141	1.000000	11.000000	3.000000	-1.0007057	1	1
143	5.000000	11.000000	3.000000	-1.5010586	0	1
145	2.000000	12.000000	3.000000	-1.5010586	1	1
147	6.000000	12.000000	3.000000	-1.5010586	0	1
149	3.000000	13.000000	3.000000	-1.5010586	0	1
151	7.000000	13.000000	3.000000	-1.5010586	0	1
153	4.000000	14.000000	3.000000	-1.5010586	1	1
155	1.000000	15.000000	3.000000	-.6254411	1	1
157	5.000000	15.000000	3.000000	-1.0007057	1	1
159	2.000000	1.000000	4.000000	-1.0007057	1	1
161	6.000000	1.000000	4.000000	-1.0007057	1	1
163	3.000000	2.000000	4.000000	-1.5010586	1	1
165	7.000000	2.000000	4.000000	-1.5010586	1	1
167	4.000000	3.000000	4.000000	-1.5010586	0	1
169	1.000000	4.000000	4.000000	-1.0007057	1	1
171	5.000000	4.000000	4.000000	-1.5010586	0	1
173	2.000000	5.000000	4.000000	-1.5010586	1	1
175	6.000000	5.000000	4.000000	-1.5010586	0	1
177	3.000000	6.000000	4.000000	-1.5010586	0	1
179	7.000000	6.000000	4.000000	-1.5010586	0	1
181	4.000000	7.000000	4.000000	-1.5010586	0	1

86	3.000000	10.000000	2.000000	-1.501059	0	1
88	7.000000	10.000000	2.000000	-1.501059	0	1
90	4.000000	11.000000	2.000000	-1.501059	0	1
92	1.000000	12.000000	2.000000	-1.000706	1	1
94	5.000000	12.000000	2.000000	-1.501059	0	1
96	2.000000	13.000000	2.000000	-1.501059	1	1
98	6.000000	13.000000	2.000000	-1.501059	0	1
100	3.000000	14.000000	2.000000	-1.501059	1	1
102	7.000000	14.000000	2.000000	-1.501059	1	1
104	4.000000	15.000000	2.000000	-1.000706	1	1
106	1.000000	1.000000	3.000000	-.625441	1	1
108	5.000000	1.000000	3.000000	-1.000706	1	1
110	2.000000	2.000000	3.000000	-1.501059	1	1
112	6.000000	2.000000	3.000000	-1.501059	1	1
114	3.000000	3.000000	3.000000	-1.501059	0	1
116	7.000000	3.000000	3.000000	-1.501059	0	1
118	4.000000	4.000000	3.000000	-1.501059	0	1
120	1.000000	5.000000	3.000000	-1.000706	1	1
122	5.000000	5.000000	3.000000	-1.501059	0	1
124	2.000000	6.000000	3.000000	-1.501059	1	1
126	6.000000	6.000000	3.000000	-1.501059	0	1
128	3.000000	7.000000	3.000000	-1.501059	0	1
130	7.000000	7.000000	3.000000	-1.501059	0	1
132	4.000000	8.000000	3.000000	-1.501059	0	1
134	1.000000	9.000000	3.000000	-1.000706	1	1
136	5.000000	9.000000	3.000000	-1.501059	0	1
138	2.000000	10.000000	3.000000	-1.501059	1	1
140	6.000000	10.000000	3.000000	-1.501059	0	1
142	3.000000	11.000000	3.000000	-1.501059	0	1
144	7.000000	11.000000	3.000000	-1.501059	0	1
146	4.000000	12.000000	3.000000	-1.501059	0	1
148	1.000000	13.000000	3.000000	-1.000706	1	1
150	5.000000	13.000000	3.000000	-1.501059	0	1
152	2.000000	14.000000	3.000000	-1.501059	1	1
154	6.000000	14.000000	3.000000	-1.501059	1	1
156	3.000000	15.000000	3.000000	-1.000706	1	1
158	7.000000	15.000000	3.000000	-1.000706	1	1
160	4.000000	1.000000	4.000000	-1.000706	1	1
162	1.000000	2.000000	4.000000	-1.000706	1	1
164	5.000000	2.000000	4.000000	-1.501059	1	1
166	2.000000	3.000000	4.000000	-1.501059	1	1
168	6.000000	3.000000	4.000000	-1.501059	0	1
170	3.000000	4.000000	4.000000	-1.501059	0	1
172	7.000000	4.000000	4.000000	-1.501059	0	1
174	4.000000	5.000000	4.000000	-1.501059	0	1
176	1.000000	6.000000	4.000000	-1.000706	1	1
178	5.000000	6.000000	4.000000	-1.501059	0	1
180	2.000000	7.000000	4.000000	-1.501059	1	1
182	6.000000	7.000000	4.000000	-1.501059	0	1

183	1.000000	8.000000	4.000000	-1.0007057	1	1	184	3.000000	8.000000	4.000000	-1.501059	0	1
185	5.000000	8.000000	4.000000	-1.5010586	0	1	186	7.000000	8.000000	4.000000	-1.501059	0	1
187	2.000000	9.000000	4.000000	-1.5010586	1	1	188	4.000000	9.000000	4.000000	-1.501059	0	1
189	6.000000	9.000000	4.000000	-1.5010586	0	1	190	1.000000	10.000000	4.000000	-1.000706	1	1
191	3.000000	10.000000	4.000000	-1.5010586	0	1	192	5.000000	10.000000	4.000000	-1.501059	0	1
193	7.000000	10.000000	4.000000	-1.5010586	0	1	194	2.000000	11.000000	4.000000	-1.501059	1	1
195	4.000000	11.000000	4.000000	-1.5010586	0	1	196	6.000000	11.000000	4.000000	-1.501059	0	1
197	1.000000	12.000000	4.000000	-1.0007057	1	1	198	3.000000	12.000000	4.000000	-1.501059	0	1
199	5.000000	12.000000	4.000000	-1.5010586	0	1	200	7.000000	12.000000	4.000000	-1.501059	0	1
201	2.000000	13.000000	4.000000	-1.5010586	1	1	202	4.000000	13.000000	4.000000	-1.501059	0	1
203	6.000000	13.000000	4.000000	-1.5010586	0	1	204	1.000000	14.000000	4.000000	-1.000706	1	1
205	3.000000	14.000000	4.000000	-1.5010586	1	1	206	5.000000	14.000000	4.000000	-1.501059	1	1
207	7.000000	14.000000	4.000000	-1.5010586	1	1	208	2.000000	15.000000	4.000000	-1.000706	1	1
209	4.000000	15.000000	4.000000	-1.0007057	1	1	210	6.000000	15.000000	4.000000	-1.000706	1	1
211	1.000000	1.625441	5.000000	-1.625441	1	1	212	3.000000	1.000000	5.000000	-1.000706	1	1
213	5.000000	1.000000	5.000000	-1.0007057	1	1	214	7.000000	1.000000	5.000000	-1.000706	1	1
215	2.000000	2.000000	5.000000	-1.5010586	1	1	216	4.000000	2.000000	5.000000	-1.501059	1	1
217	6.000000	2.000000	5.000000	-1.5010586	1	1	218	1.000000	3.000000	5.000000	-1.000706	1	1
219	3.000000	3.000000	5.000000	-1.5010586	0	1	220	5.000000	3.000000	5.000000	-1.501059	0	1
221	7.000000	3.000000	5.000000	-1.5010586	0	1	222	2.000000	4.000000	5.000000	-1.501059	1	1
223	4.000000	4.000000	5.000000	-1.5010586	0	1	224	6.000000	4.000000	5.000000	-1.501059	0	1
225	1.000000	5.000000	5.000000	-1.0007057	1	1	226	3.000000	5.000000	5.000000	-1.501059	0	1
227	5.000000	5.000000	5.000000	-1.5010586	0	1	228	7.000000	5.000000	5.000000	-1.501059	0	1
229	2.000000	6.000000	5.000000	-1.5010586	1	1	230	4.000000	6.000000	5.000000	-1.501059	0	1
231	6.000000	6.000000	5.000000	-1.5010586	0	1	232	1.000000	7.000000	5.000000	-1.000706	1	1
233	3.000000	7.000000	5.000000	-1.5010586	0	1	234	5.000000	7.000000	5.000000	-1.501059	0	1
235	7.000000	7.000000	5.000000	-1.5010586	0	1	236	2.000000	8.000000	5.000000	-1.501059	1	1
237	4.000000	8.000000	5.000000	-1.5010586	0	1	238	6.000000	8.000000	5.000000	-1.501059	0	1
239	1.000000	9.000000	5.000000	-1.0007057	1	1	240	3.000000	9.000000	5.000000	-1.501059	0	1
241	5.000000	9.000000	5.000000	-1.5010586	0	1	242	7.000000	9.000000	5.000000	-1.501059	0	1
243	2.000000	10.000000	5.000000	-1.5010586	1	1	244	4.000000	10.000000	5.000000	-1.501059	0	1
245	6.000000	10.000000	5.000000	-1.5010586	0	1	246	1.000000	11.000000	5.000000	-1.000706	1	1
247	3.000000	11.000000	5.000000	-1.5010586	0	1	248	5.000000	11.000000	5.000000	-1.501059	0	1
249	7.000000	11.000000	5.000000	-1.5010586	0	1	250	2.000000	12.000000	5.000000	-1.501059	1	1
251	4.000000	12.000000	5.000000	-1.5010586	0	1	252	6.000000	12.000000	5.000000	-1.501059	0	1
253	1.000000	13.000000	5.000000	-1.0007057	1	1	254	3.000000	13.000000	5.000000	-1.501059	0	1
255	5.000000	13.000000	5.000000	-1.5010586	0	1	256	7.000000	13.000000	5.000000	-1.501059	0	1
257	2.000000	14.000000	5.000000	-1.5010586	1	1	258	4.000000	14.000000	5.000000	-1.501059	1	1
259	6.000000	14.000000	5.000000	-1.5010586	1	1	260	1.000000	15.000000	5.000000	-1.000706	1	1
261	3.000000	15.000000	5.000000	-1.0007057	1	1	262	5.000000	15.000000	5.000000	-1.000706	1	1
263	7.000000	15.000000	5.000000	-1.0007057	1	1	264	2.000000	1.000000	6.000000	-1.000706	1	1
265	4.000000	1.000000	6.000000	-1.0007057	1	1	266	6.000000	1.000000	6.000000	-1.000706	1	1
267	1.000000	2.000000	6.000000	-1.0007057	1	1	268	3.000000	2.000000	6.000000	-1.501059	1	1
269	5.000000	2.000000	6.000000	-1.5010586	1	1	270	7.000000	2.000000	6.000000	-1.501059	1	1
271	2.000000	3.000000	6.000000	-1.5010586	1	1	272	4.000000	3.000000	6.000000	-1.501059	0	1
273	6.000000	3.000000	6.000000	-1.5010586	0	1	274	1.000000	4.000000	6.000000	-1.000706	1	1
275	3.000000	4.000000	6.000000	-1.5010586	0	1	276	5.000000	4.000000	6.000000	-1.501059	0	1
277	7.000000	4.000000	6.000000	-1.5010586	0	1	278	2.000000	5.000000	6.000000	-1.501059	1	1
279	4.000000	5.000000	6.000000	-1.5010586	0	1	280	6.000000	5.000000	6.000000	-1.501059	0	1

281	1.000000	6.000000	6.000000	-1.0007057	1	1	282	3.000000	6.000000	6.000000	-1.501059	0	1
283	5.000000	6.000000	6.000000	-1.5010586	0	1	284	7.000000	6.000000	6.000000	-1.501059	0	1
285	2.000000	7.000000	6.000000	-1.5010586	1	1	286	4.000000	7.000000	6.000000	-1.501059	0	1
287	6.000000	7.000000	6.000000	-1.5010586	0	1	288	1.000000	8.000000	6.000000	-1.000706	1	1
289	3.000000	8.000000	6.000000	-1.5010586	0	1	290	5.000000	8.000000	6.000000	-1.501059	0	1
291	7.000000	8.000000	6.000000	-1.5010586	0	1	292	2.000000	9.000000	6.000000	-1.501059	1	1
293	4.000000	9.000000	6.000000	-1.5010586	0	1	294	6.000000	9.000000	6.000000	-1.501059	0	1
295	1.000000	10.000000	6.000000	-1.0007057	1	1	296	3.000000	10.000000	6.000000	-1.501059	0	1
297	5.000000	10.000000	6.000000	-1.5010586	0	1	298	7.000000	10.000000	6.000000	-1.501059	0	1
299	2.000000	11.000000	6.000000	-1.5010586	1	1	300	4.000000	11.000000	6.000000	-1.501059	0	1
301	6.000000	11.000000	6.000000	-1.5010586	0	1	302	1.000000	12.000000	6.000000	-1.000706	1	1
303	3.000000	12.000000	6.000000	-1.5010586	0	1	304	5.000000	12.000000	6.000000	-1.501059	0	1
305	7.000000	12.000000	6.000000	-1.5010586	0	1	306	2.000000	13.000000	6.000000	-1.501059	1	1
307	4.000000	13.000000	6.000000	-1.5010586	0	1	308	6.000000	13.000000	6.000000	-1.501059	0	1
309	1.000000	14.000000	6.000000	-1.0007057	1	1	310	3.000000	14.000000	6.000000	-1.501059	1	1
311	5.000000	14.000000	6.000000	-1.5010586	1	1	312	7.000000	14.000000	6.000000	-1.501059	1	1
313	2.000000	15.000000	6.000000	-1.0007057	1	1	314	4.000000	15.000000	6.000000	-1.000706	1	1
315	6.000000	15.000000	6.000000	-1.0007057	1	1	316	1.000000	1.000000	7.000000	-.375265	1	1
317	3.000000	1.000000	7.000000	-.6254411	1	1	318	5.000000	1.000000	7.000000	-.625441	1	1
319	7.000000	1.000000	7.000000	-.6254411	1	1	320	2.000000	2.000000	7.000000	-1.000706	1	1
321	4.000000	2.000000	7.000000	-1.0007057	1	1	322	6.000000	2.000000	7.000000	-1.000706	1	1
323	1.000000	3.000000	7.000000	-.6254411	1	1	324	3.000000	3.000000	7.000000	-1.000706	0	1
325	5.000000	3.000000	7.000000	-1.0007057	0	1	326	7.000000	3.000000	7.000000	-1.000706	0	1
327	2.000000	4.000000	7.000000	-1.0007057	1	1	328	4.000000	4.000000	7.000000	-1.000706	0	1
329	6.000000	4.000000	7.000000	-1.0007057	0	1	330	1.000000	5.000000	7.000000	-.625441	1	1
331	3.000000	5.000000	7.000000	-1.0007057	0	1	332	5.000000	5.000000	7.000000	-1.000706	0	1
333	7.000000	5.000000	7.000000	-1.0007057	0	1	334	2.000000	6.000000	7.000000	-1.000706	1	1
335	4.000000	6.000000	7.000000	-1.0007057	0	1	336	6.000000	6.000000	7.000000	-1.000706	0	1
337	1.000000	7.000000	7.000000	-.6254411	1	1	338	3.000000	7.000000	7.000000	-1.000706	0	1
339	5.000000	7.000000	7.000000	-1.0007057	0	1	340	7.000000	7.000000	7.000000	-1.000706	0	1
341	2.000000	8.000000	7.000000	-1.0007057	1	1	342	4.000000	8.000000	7.000000	-1.000706	0	1
343	6.000000	8.000000	7.000000	-1.0007057	0	1	344	1.000000	9.000000	7.000000	-.625441	1	1
345	3.000000	9.000000	7.000000	-1.0007057	0	1	346	5.000000	9.000000	7.000000	-1.000706	0	1
347	7.000000	9.000000	7.000000	-1.0007057	0	1	348	2.000000	10.000000	7.000000	-1.000706	1	1
349	4.000000	10.000000	7.000000	-1.0007057	0	1	350	6.000000	10.000000	7.000000	-1.000706	0	1
351	1.000000	11.000000	7.000000	-.6254411	1	1	352	3.000000	11.000000	7.000000	-1.000706	0	1
353	5.000000	11.000000	7.000000	-1.0007057	0	1	354	7.000000	11.000000	7.000000	-1.000706	0	1
355	2.000000	12.000000	7.000000	-1.0007057	1	1	356	4.000000	12.000000	7.000000	-1.000706	0	1
357	6.000000	12.000000	7.000000	-1.0007057	0	1	358	1.000000	13.000000	7.000000	-.625441	1	1
359	3.000000	13.000000	7.000000	-1.0007057	0	1	360	5.000000	13.000000	7.000000	-1.000706	0	1
361	7.000000	13.000000	7.000000	-1.0007057	0	1	362	2.000000	14.000000	7.000000	-1.000706	1	1
363	4.000000	14.000000	7.000000	-1.0007057	1	1	364	6.000000	14.000000	7.000000	-1.000706	1	1
365	1.000000	15.000000	7.000000	-.3752646	1	1	366	3.000000	15.000000	7.000000	-.625441	1	1
367	5.000000	15.000000	7.000000	-.6254411	1	1	368	7.000000	15.000000	7.000000	-.625441	1	1
369	2.000000	1.000000	1.000000	-.6254411	1	1	370	11.000000	1.000000	1.000000	-.625441	1	1
371	13.000000	1.000000	1.000000	-.6254411	1	1	372	15.000000	1.000000	1.000000	-.375265	1	1
373	8.000000	2.000000	1.000000	-1.0007057	1	1	374	10.000000	2.000000	1.000000	-1.000706	1	1
375	12.000000	2.000000	1.000000	-1.0007057	1	1	376	14.000000	2.000000	1.000000	-1.000706	1	1
377	9.000000	3.000000	1.000000	-1.0007057	0	1	378	11.000000	3.000000	1.000000	-1.000706	0	1

376	13.000000	3.000000	1.000000	-1.0007057	0	1	380	15.000000	3.000000	1.000000	-.625441	1	1
381	3.000000	4.000000	1.000000	-1.0007057	0	1	382	10.000000	4.000000	1.000000	-1.000706	0	1
383	12.000000	4.000000	1.000000	-1.0007057	0	1	384	14.000000	4.000000	1.000000	-1.000706	1	1
385	9.000000	5.000000	1.000000	-1.0007057	0	1	386	11.000000	5.000000	1.000000	-1.000706	0	1
387	15.000000	5.000000	1.000000	-1.0007057	0	1	388	15.000000	5.000000	1.000000	-.625441	1	1
389	6.000000	6.000000	1.000000	-1.0007057	0	1	390	10.000000	6.000000	1.000000	-1.000706	0	1
391	12.000000	6.000000	1.000000	-1.0007057	0	1	392	14.000000	6.000000	1.000000	-1.000706	1	1
393	9.000000	7.000000	1.000000	-1.0007057	0	1	394	11.000000	7.000000	1.000000	-1.000706	0	1
395	15.000000	7.000000	1.000000	-1.0007057	0	1	396	15.000000	7.000000	1.000000	-.625441	1	1
397	3.000000	8.000000	1.000000	-1.0007057	0	1	398	10.000000	8.000000	1.000000	-1.000706	0	1
399	12.000000	8.000000	1.000000	-1.0007057	0	1	400	14.000000	8.000000	1.000000	-1.000706	1	1
401	9.000000	9.000000	1.000000	-1.0007057	0	1	402	11.000000	9.000000	1.000000	-1.000706	0	1
403	15.000000	9.000000	1.000000	-1.0007057	0	1	404	15.000000	9.000000	1.000000	-.625441	1	1
405	3.000000	10.000000	1.000000	-1.0007057	0	1	406	10.000000	10.000000	1.000000	-1.000706	0	1
407	12.000000	10.000000	1.000000	-1.0007057	0	1	408	14.000000	10.000000	1.000000	-1.000706	1	1
409	9.000000	11.000000	1.000000	-1.0007057	0	1	410	11.000000	11.000000	1.000000	-1.000706	0	1
411	15.000000	11.000000	1.000000	-1.0007057	0	1	412	15.000000	11.000000	1.000000	-.625441	1	1
413	3.000000	12.000000	1.000000	-1.0007057	0	1	414	10.000000	12.000000	1.000000	-1.000706	0	1
415	12.000000	12.000000	1.000000	-1.0007057	0	1	416	14.000000	12.000000	1.000000	-1.000706	1	1
417	9.000000	13.000000	1.000000	-1.0007057	0	1	418	11.000000	13.000000	1.000000	-1.000706	0	1
419	15.000000	13.000000	1.000000	-1.0007057	0	1	420	15.000000	13.000000	1.000000	-.625441	1	1
421	3.000000	14.000000	1.000000	-1.0007057	1	1	422	10.000000	14.000000	1.000000	-1.000706	1	1
423	12.000000	14.000000	1.000000	-1.0007057	1	1	424	14.000000	14.000000	1.000000	-1.000706	1	1
425	9.000000	15.000000	1.000000	-.625441	1	1	426	11.000000	15.000000	1.000000	-.625441	1	1
427	15.000000	15.000000	1.000000	-.625441	1	1	428	15.000000	15.000000	1.000000	-.375265	1	1
429	3.000000	1.000000	2.000000	-1.0007057	1	1	430	10.000000	1.000000	2.000000	-1.000706	1	1
431	12.000000	1.000000	2.000000	-1.0007057	1	1	432	14.000000	1.000000	2.000000	-1.000706	1	1
433	9.000000	2.000000	2.000000	-1.5010586	1	1	434	11.000000	2.000000	2.000000	-1.501059	1	1
435	15.000000	2.000000	2.000000	-1.5010586	1	1	436	15.000000	2.000000	2.000000	-1.000706	1	1
437	3.000000	3.000000	2.000000	-1.5010586	0	1	438	10.000000	3.000000	2.000000	-1.501059	0	1
439	12.000000	3.000000	2.000000	-1.5010586	0	1	440	14.000000	3.000000	2.000000	-1.501059	1	1
441	9.000000	4.000000	2.000000	-1.5010586	0	1	442	11.000000	4.000000	2.000000	-1.501059	0	1
443	15.000000	4.000000	2.000000	-1.5010586	0	1	444	15.000000	4.000000	2.000000	-1.000706	1	1
445	3.000000	5.000000	2.000000	-1.5010586	0	1	446	10.000000	5.000000	2.000000	-1.501059	0	1
447	12.000000	5.000000	2.000000	-1.5010586	0	1	448	14.000000	5.000000	2.000000	-1.501059	1	1
449	9.000000	6.000000	2.000000	-1.5010586	0	1	450	11.000000	6.000000	2.000000	-1.501059	0	1
451	15.000000	6.000000	2.000000	-1.5010586	0	1	452	15.000000	6.000000	2.000000	-1.000706	1	1
453	3.000000	7.000000	2.000000	-1.5010586	0	1	454	10.000000	7.000000	2.000000	-1.501059	0	1
455	12.000000	7.000000	2.000000	-1.5010586	0	1	456	14.000000	7.000000	2.000000	-1.501059	1	1
457	9.000000	8.000000	2.000000	-1.5010586	0	1	458	11.000000	8.000000	2.000000	-1.501059	0	1
459	15.000000	8.000000	2.000000	-1.5010586	0	1	460	15.000000	8.000000	2.000000	-1.000706	1	1
461	3.000000	9.000000	2.000000	-1.5010586	0	1	462	10.000000	9.000000	2.000000	-1.501059	0	1
463	12.000000	9.000000	2.000000	-1.5010586	0	1	464	14.000000	9.000000	2.000000	-1.501059	1	1
465	9.000000	10.000000	2.000000	-1.5010586	0	1	466	11.000000	10.000000	2.000000	-1.501059	0	1
467	15.000000	10.000000	2.000000	-1.5010586	0	1	468	15.000000	10.000000	2.000000	-1.000706	1	1
469	3.000000	11.000000	2.000000	-1.5010586	0	1	470	10.000000	11.000000	2.000000	-1.501059	0	1
471	12.000000	11.000000	2.000000	-1.5010586	0	1	472	14.000000	11.000000	2.000000	-1.501059	1	1
473	9.000000	12.000000	2.000000	-1.5010586	0	1	474	11.000000	12.000000	2.000000	-1.501059	0	1
475	15.000000	12.000000	2.000000	-1.5010586	0	1	476	15.000000	12.000000	2.000000	-1.000706	1	1

477	8.000000	13.000000	2.000000	-1.5010586	0	1
479	12.000000	13.000000	2.000000	-1.5010586	0	1
481	9.000000	14.000000	2.000000	-1.5010586	1	1
483	13.000000	14.000000	2.000000	-1.5010586	1	1
485	8.000000	15.000000	2.000000	-1.0007057	1	1
487	12.000000	15.000000	2.000000	-1.0007057	1	1
489	9.000000	1.000000	3.000000	-1.0007057	1	1
491	13.000000	1.000000	3.000000	-1.0007057	1	1
493	8.000000	2.000000	3.000000	-1.5010586	1	1
495	12.000000	2.000000	3.000000	-1.5010586	1	1
497	9.000000	3.000000	3.000000	-1.5010586	0	1
499	13.000000	3.000000	3.000000	-1.5010586	0	1
501	8.000000	4.000000	3.000000	-1.5010586	0	1
503	12.000000	4.000000	3.000000	-1.5010586	0	1
505	9.000000	5.000000	3.000000	-1.5010586	0	1
507	13.000000	5.000000	3.000000	-1.5010586	0	1
509	8.000000	6.000000	3.000000	-1.5010586	0	1
511	12.000000	6.000000	3.000000	-1.5010586	0	1
513	9.000000	7.000000	3.000000	-1.5010586	0	1
515	13.000000	7.000000	3.000000	-1.5010586	0	1
517	8.000000	8.000000	3.000000	-1.5010586	0	1
519	12.000000	8.000000	3.000000	-1.5010586	0	1
521	9.000000	9.000000	3.000000	-1.5010586	0	1
523	13.000000	9.000000	3.000000	-1.5010586	0	1
525	8.000000	10.000000	3.000000	-1.5010586	0	1
527	12.000000	10.000000	3.000000	-1.5010586	0	1
529	9.000000	11.000000	3.000000	-1.5010586	0	1
531	13.000000	11.000000	3.000000	-1.5010586	0	1
533	8.000000	12.000000	3.000000	-1.5010586	0	1
535	12.000000	12.000000	3.000000	-1.5010586	0	1
537	9.000000	13.000000	3.000000	-1.5010586	0	1
539	13.000000	13.000000	3.000000	-1.5010586	0	1
541	8.000000	14.000000	3.000000	-1.5010586	1	1
543	12.000000	14.000000	3.000000	-1.5010586	1	1
545	9.000000	15.000000	3.000000	-1.0007057	1	1
547	13.000000	15.000000	3.000000	-1.0007057	1	1
549	8.000000	1.000000	4.000000	-1.0007057	1	1
551	12.000000	1.000000	4.000000	-1.0007057	1	1
553	9.000000	2.000000	4.000000	-1.5010586	1	1
555	13.000000	2.000000	4.000000	-1.5010586	1	1
557	8.000000	3.000000	4.000000	-1.5010586	0	1
559	12.000000	3.000000	4.000000	-1.5010586	0	1
561	9.000000	4.000000	4.000000	-1.5010586	0	1
563	13.000000	4.000000	4.000000	-1.5010586	0	1
565	8.000000	5.000000	4.000000	-1.5010586	0	1
567	12.000000	5.000000	4.000000	-1.5010586	0	1
569	9.000000	6.000000	4.000000	-1.5010586	0	1
571	13.000000	6.000000	4.000000	-1.5010586	0	1
573	8.000000	7.000000	4.000000	-1.5010586	0	1

478	10.000000	13.000000	2.000000	-1.501059	0	1
480	14.000000	13.000000	2.000000	-1.501059	1	1
482	11.000000	14.000000	2.000000	-1.501059	1	1
484	15.000000	14.000000	2.000000	-1.000706	1	1
486	10.000000	15.000000	2.000000	-1.000706	1	1
488	14.000000	15.000000	2.000000	-1.000706	1	1
490	11.000000	1.000000	3.000000	-1.000706	1	1
492	15.000000	1.000000	3.000000	-.625441	1	1
494	10.000000	2.000000	9.000000	-1.501059	1	1
496	14.000000	2.000000	3.000000	-1.501059	1	1
498	11.000000	3.000000	3.000000	-1.501059	0	1
500	15.000000	3.000000	3.000000	-1.000706	1	1
502	10.000000	4.000000	3.000000	-1.501059	0	1
504	14.000000	4.000000	3.000000	-1.501059	1	1
506	11.000000	5.000000	3.000000	-1.501059	0	1
508	15.000000	5.000000	3.000000	-1.000706	1	1
510	10.000000	6.000000	3.000000	-1.501059	0	1
512	14.000000	6.000000	3.000000	-1.501059	1	1
514	11.000000	7.000000	3.000000	-1.501059	0	1
516	15.000000	7.000000	3.000000	-1.000706	1	1
518	10.000000	8.000000	3.000000	-1.501059	0	1
520	14.000000	8.000000	3.000000	-1.501059	1	1
522	11.000000	9.000000	3.000000	-1.501059	0	1
524	15.000000	9.000000	3.000000	-1.000706	1	1
526	10.000000	10.000000	3.000000	-1.501059	0	1
528	14.000000	10.000000	3.000000	-1.501059	1	1
530	11.000000	11.000000	3.000000	-1.501059	0	1
532	15.000000	11.000000	3.000000	-1.000706	1	1
534	10.000000	12.000000	3.000000	-1.501059	0	1
536	14.000000	12.000000	3.000000	-1.501059	1	1
538	11.000000	13.000000	3.000000	-1.501059	0	1
540	15.000000	13.000000	3.000000	-1.000706	1	1
542	10.000000	14.000000	3.000000	-1.501059	1	1
544	14.000000	14.000000	3.000000	-1.501059	1	1
546	11.000000	15.000000	3.000000	-1.000706	1	1
548	15.000000	15.000000	3.000000	-.625441	1	1
550	10.000000	1.000000	4.000000	-1.000706	1	1
552	14.000000	1.000000	4.000000	-1.000706	1	1
554	11.000000	2.000000	4.000000	-1.501059	1	1
556	15.000000	2.000000	4.000000	-1.000706	1	1
558	10.000000	3.000000	4.000000	-1.501059	0	1
560	14.000000	3.000000	4.000000	-1.501059	1	1
562	11.000000	4.000000	4.000000	-1.501059	0	1
564	15.000000	4.000000	4.000000	-1.000706	1	1
566	10.000000	5.000000	4.000000	-1.501059	0	1
568	14.000000	5.000000	4.000000	-1.501059	1	1
570	11.000000	6.000000	4.000000	-1.501059	0	1
572	15.000000	6.000000	4.000000	-1.000706	1	1
574	10.000000	7.000000	4.000000	-1.501059	0	1

575	12.000000	7.000000	4.000000	-1.5010586	0	1	576	14.000000	7.000000	4.000000	-1.501059	1	1
577	8.000000	8.000000	4.000000	-1.5010586	0	1	578	11.000000	8.000000	4.000000	-1.501059	0	1
579	13.000000	8.000000	4.000000	-1.5010586	0	1	580	15.000000	8.000000	4.000000	-1.000706	1	1
581	8.000000	9.000000	4.000000	-1.5010586	0	1	582	10.000000	9.000000	4.000000	-1.501059	0	1
583	12.000000	9.000000	4.000000	-1.5010586	0	1	584	14.000000	9.000000	4.000000	-1.501059	1	1
585	9.000000	10.000000	4.000000	-1.5010586	0	1	586	11.000000	10.000000	4.000000	-1.501059	0	1
587	13.000000	10.000000	4.000000	-1.5010586	0	1	588	15.000000	10.000000	4.000000	-1.000706	1	1
589	8.000000	11.000000	4.000000	-1.5010586	0	1	590	10.000000	11.000000	4.000000	-1.501059	0	1
591	12.000000	11.000000	4.000000	-1.5010586	0	1	592	14.000000	11.000000	4.000000	-1.501059	1	1
593	9.000000	12.000000	4.000000	-1.5010586	0	1	594	11.000000	12.000000	4.000000	-1.501059	0	1
595	13.000000	12.000000	4.000000	-1.5010586	0	1	596	15.000000	12.000000	4.000000	-1.000706	1	1
597	8.000000	13.000000	4.000000	-1.5010586	0	1	598	10.000000	13.000000	4.000000	-1.501059	0	1
599	12.000000	13.000000	4.000000	-1.5010586	0	1	600	14.000000	13.000000	4.000000	-1.501059	1	1
601	9.000000	14.000000	4.000000	-1.5010586	1	1	602	11.000000	14.000000	4.000000	-1.501059	1	1
603	13.000000	14.000000	4.000000	-1.5010586	1	1	604	15.000000	14.000000	4.000000	-1.000706	1	1
605	8.000000	15.000000	4.000000	-1.0007057	1	1	606	10.000000	15.000000	4.000000	-1.000706	1	1
607	12.000000	15.000000	4.000000	-1.0007057	1	1	608	14.000000	15.000000	4.000000	-1.000706	1	1
609	9.000000	1.000000	5.000000	-1.0007057	1	1	610	11.000000	1.000000	5.000000	-1.000706	1	1
611	13.000000	1.000000	5.000000	-1.0007057	1	1	612	15.000000	1.000000	5.000000	-.625441	1	1
613	8.000000	2.000000	5.000000	-1.5010586	1	1	614	10.000000	2.000000	5.000000	-1.501059	1	1
615	12.000000	2.000000	5.000000	-1.5010586	1	1	616	14.000000	2.000000	5.000000	-1.501059	1	1
617	9.000000	3.000000	5.000000	-1.5010586	0	1	618	11.000000	3.000000	5.000000	-1.501059	0	1
619	13.000000	3.000000	5.000000	-1.5010586	0	1	620	15.000000	3.000000	5.000000	-1.000706	1	1
621	8.000000	4.000000	5.000000	-1.5010586	0	1	622	10.000000	4.000000	5.000000	-1.501059	0	1
623	12.000000	4.000000	5.000000	-1.5010586	0	1	624	14.000000	4.000000	5.000000	-1.501059	1	1
625	9.000000	5.000000	5.000000	-1.5010586	0	1	626	11.000000	5.000000	5.000000	-1.501059	0	1
627	13.000000	5.000000	5.000000	-1.5010586	0	1	628	15.000000	5.000000	5.000000	-1.000706	1	1
629	8.000000	6.000000	5.000000	-1.5010586	0	1	630	10.000000	6.000000	5.000000	-1.501059	0	1
631	12.000000	6.000000	5.000000	-1.5010586	0	1	632	14.000000	6.000000	5.000000	-1.501059	1	1
633	9.000000	7.000000	5.000000	-1.5010586	0	1	634	11.000000	7.000000	5.000000	-1.501059	0	1
635	13.000000	7.000000	5.000000	-1.5010586	0	1	636	15.000000	7.000000	5.000000	-1.000706	1	1
637	8.000000	8.000000	5.000000	-1.5010586	0	1	638	10.000000	8.000000	5.000000	-1.501059	0	1
639	12.000000	8.000000	5.000000	-1.5010586	0	1	640	14.000000	8.000000	5.000000	-1.501059	1	1
641	9.000000	9.000000	5.000000	-1.5010586	0	1	642	11.000000	9.000000	5.000000	-1.501059	0	1
643	13.000000	9.000000	5.000000	-1.5010586	0	1	644	15.000000	9.000000	5.000000	-1.000706	1	1
645	8.000000	10.000000	5.000000	-1.5010586	0	1	646	10.000000	10.000000	5.000000	-1.501059	0	1
647	12.000000	10.000000	5.000000	-1.5010586	0	1	648	14.000000	10.000000	5.000000	-1.501059	1	1
649	9.000000	11.000000	5.000000	-1.5010586	0	1	650	11.000000	11.000000	5.000000	-1.501059	0	1
651	13.000000	11.000000	5.000000	-1.5010586	0	1	652	15.000000	11.000000	5.000000	-1.000706	1	1
653	8.000000	12.000000	5.000000	-1.5010586	0	1	654	10.000000	12.000000	5.000000	-1.501059	0	1
655	12.000000	12.000000	5.000000	-1.5010586	0	1	656	14.000000	12.000000	5.000000	-1.501059	1	1
657	9.000000	13.000000	5.000000	-1.5010586	0	1	658	11.000000	13.000000	5.000000	-1.501059	0	1
659	13.000000	13.000000	5.000000	-1.5010586	0	1	660	15.000000	13.000000	5.000000	-1.000706	1	1
661	8.000000	14.000000	5.000000	-1.5010586	1	1	662	10.000000	14.000000	5.000000	-1.501059	1	1
663	12.000000	14.000000	5.000000	-1.5010586	1	1	664	14.000000	14.000000	5.000000	-1.501059	1	1
665	9.000000	15.000000	5.000000	-1.0007057	1	1	666	11.000000	15.000000	5.000000	-1.000706	1	1
667	13.000000	15.000000	5.000000	-1.0007057	1	1	668	15.000000	15.000000	5.000000	-.625441	1	1
669	8.000000	1.000000	6.000000	-1.0007057	1	1	670	10.000000	1.000000	6.000000	-1.000706	1	1
671	12.000000	1.000000	6.000000	-1.0007057	1	1	672	14.000000	1.000000	6.000000	-1.000706	1	1

673	9.000000	2.000000	6.000000	-1.5010586	1	1	674	11.000000	2.000000	6.000000	-1.501059	1	1
675	13.000000	2.000000	6.000000	-1.5010586	1	1	676	15.000000	2.000000	6.000000	-1.000706	1	1
677	8.000000	3.000000	6.000000	-1.5010586	0	1	678	10.000000	3.000000	6.000000	-1.501059	0	1
679	12.000000	3.000000	6.000000	-1.5010586	0	1	680	14.000000	3.000000	6.000000	-1.501059	1	1
681	9.000000	4.000000	6.000000	-1.5010586	0	1	682	11.000000	4.000000	6.000000	-1.501059	0	1
683	13.000000	4.000000	6.000000	-1.5010586	0	1	684	15.000000	4.000000	6.000000	-1.000706	1	1
685	8.000000	5.000000	6.000000	-1.5010586	0	1	686	10.000000	5.000000	6.000000	-1.501059	0	1
687	12.000000	5.000000	6.000000	-1.5010586	0	1	688	14.000000	5.000000	6.000000	-1.501059	1	1
689	9.000000	6.000000	6.000000	-1.5010586	0	1	690	11.000000	6.000000	6.000000	-1.501059	0	1
691	13.000000	6.000000	6.000000	-1.5010586	0	1	692	15.000000	6.000000	6.000000	-1.000706	1	1
693	8.000000	7.000000	6.000000	-1.5010586	0	1	694	10.000000	7.000000	6.000000	-1.501059	0	1
695	12.000000	7.000000	6.000000	-1.5010586	0	1	696	14.000000	7.000000	6.000000	-1.501059	1	1
697	9.000000	8.000000	6.000000	-1.5010586	0	1	698	11.000000	8.000000	6.000000	-1.501059	0	1
699	13.000000	8.000000	6.000000	-1.5010586	0	1	700	15.000000	8.000000	6.000000	-1.000706	1	1
701	8.000000	9.000000	6.000000	-1.5010586	0	1	702	10.000000	9.000000	6.000000	-1.501059	0	1
703	12.000000	9.000000	6.000000	-1.5010586	0	1	704	14.000000	9.000000	6.000000	-1.501059	1	1
705	9.000000	10.000000	6.000000	-1.5010586	0	1	706	11.000000	10.000000	6.000000	-1.501059	0	1
707	13.000000	10.000000	6.000000	-1.5010586	0	1	708	15.000000	10.000000	6.000000	-1.000706	1	1
709	8.000000	11.000000	6.000000	-1.5010586	0	1	710	10.000000	11.000000	6.000000	-1.501059	0	1
711	12.000000	11.000000	6.000000	-1.5010586	0	1	712	14.000000	11.000000	6.000000	-1.501059	1	1
713	9.000000	12.000000	6.000000	-1.5010586	0	1	714	11.000000	12.000000	6.000000	-1.501059	0	1
715	13.000000	12.000000	6.000000	-1.5010586	0	1	716	15.000000	12.000000	6.000000	-1.000706	1	1
717	8.000000	13.000000	6.000000	-1.5010586	0	1	718	10.000000	13.000000	6.000000	-1.501059	0	1
719	12.000000	13.000000	6.000000	-1.5010586	0	1	720	14.000000	13.000000	6.000000	-1.501059	1	1
721	9.000000	14.000000	6.000000	-1.5010586	1	1	722	11.000000	14.000000	6.000000	-1.501059	1	1
723	13.000000	14.000000	6.000000	-1.5010586	1	1	724	15.000000	14.000000	6.000000	-1.000706	1	1
725	8.000000	15.000000	6.000000	-1.0007057	1	1	726	10.000000	15.000000	6.000000	-1.000706	1	1
727	12.000000	15.000000	6.000000	-1.0007057	1	1	728	14.000000	15.000000	6.000000	-1.000706	1	1
729	9.000000	1.000000	7.000000	-.625441	1	1	730	11.000000	1.000000	7.000000	-.625441	1	1
731	13.000000	1.000000	7.000000	-.625441	1	1	732	15.000000	1.000000	7.000000	-.375265	1	1
733	8.000000	2.000000	7.000000	-1.0007057	1	1	734	10.000000	2.000000	7.000000	-1.000706	1	1
735	12.000000	2.000000	7.000000	-1.0007057	1	1	736	14.000000	2.000000	7.000000	-1.000706	1	1
737	9.000000	3.000000	7.000000	-1.0007057	0	1	738	11.000000	3.000000	7.000000	-1.000706	0	1
739	13.000000	3.000000	7.000000	-1.0007057	0	1	740	15.000000	3.000000	7.000000	-.625441	1	1
741	8.000000	4.000000	7.000000	-1.0007057	0	1	742	10.000000	4.000000	7.000000	-1.000706	0	1
743	12.000000	4.000000	7.000000	-1.0007057	0	1	744	14.000000	4.000000	7.000000	-1.000706	1	1
745	9.000000	5.000000	7.000000	-1.0007057	0	1	746	11.000000	5.000000	7.000000	-1.000706	0	1
747	13.000000	5.000000	7.000000	-1.0007057	0	1	748	15.000000	5.000000	7.000000	-.625441	1	1
749	8.000000	6.000000	7.000000	-1.0007057	0	1	750	10.000000	6.000000	7.000000	-1.000706	0	1
751	12.000000	6.000000	7.000000	-1.0007057	0	1	752	14.000000	6.000000	7.000000	-1.000706	1	1
753	9.000000	7.000000	7.000000	-1.0007057	0	1	754	11.000000	7.000000	7.000000	-1.000706	0	1
755	13.000000	7.000000	7.000000	-1.0007057	0	1	756	15.000000	7.000000	7.000000	-.625441	1	1
757	8.000000	8.000000	7.000000	-1.0007057	0	1	758	10.000000	8.000000	7.000000	-1.000706	0	1
759	12.000000	8.000000	7.000000	-1.0007057	0	1	760	14.000000	8.000000	7.000000	-1.000706	1	1
761	9.000000	9.000000	7.000000	-1.0007057	0	1	762	11.000000	9.000000	7.000000	-1.000706	0	1
763	13.000000	9.000000	7.000000	-1.0007057	0	1	764	15.000000	9.000000	7.000000	-.625441	1	1
765	8.000000	10.000000	7.000000	-1.0007057	0	1	766	10.000000	10.000000	7.000000	-1.000706	0	1
767	12.000000	10.000000	7.000000	-1.0007057	0	1	768	14.000000	10.000000	7.000000	-1.000706	1	1
769	9.000000	11.000000	7.000000	-1.0007057	0	1	770	11.000000	11.000000	7.000000	-1.000706	0	1

771	13.000000	11.000000	7.000000	-1.0007057	0	1
773	8.000000	12.000000	7.000000	-1.0007057	0	1
775	12.000000	12.000000	7.000000	-1.0007057	0	1
777	9.000000	13.000000	7.000000	-1.0007057	0	1
779	13.000000	13.000000	7.000000	-1.0007057	0	1
781	8.000000	14.000000	7.000000	-1.0007057	1	1
783	12.000000	14.000000	7.000000	-1.0007057	1	1
785	9.000000	15.000000	7.000000	-.6254411	1	1
787	13.000000	15.000000	7.000000	-.6254411	1	1

772	15.000000	11.000000	7.000000	-.625441	1	1
774	10.000000	12.000000	7.000000	-1.000706	0	1
776	14.000000	12.000000	7.000000	-1.000706	1	1
778	11.000000	13.000000	7.000000	-1.000706	0	1
780	15.000000	13.000000	7.000000	-.625441	1	1
782	10.000000	14.000000	7.000000	-1.000706	1	1
784	14.000000	14.000000	7.000000	-1.000706	1	1
786	11.000000	15.000000	7.000000	-.625441	1	1
788	15.000000	15.000000	7.000000	-.375265	1	1

TIME	POTENTIAL ENERGY	KINETIC ENERGY	TOTAL ENERGY	MAXIMUM KINETIC ENERGY	SURFACE ENERGY (eV)
1.000	-974.812120	3.5991150-01	-974.452210	2.9414238-01 (789)	-398.280730
2.000	-975.044550	3.1438593-01	-974.730160	1.7472980-01 (789)	-398.280730
3.000	-975.044550	2.8314200-01	-974.761410	2.3057086-01 (789)	-398.280730
4.000	-975.107820	1.7680958-01	-974.991020	1.4647448-01 (789)	-398.280730
5.000	-975.167820	2.1276722-01	-974.955050	1.8614815-01 (789)	-398.280730
6.000	-975.306090	1.1135978-01	-975.194720	8.3429021-02 (789)	-398.280730
7.000	-975.306090	1.5439670-01	-975.151690	1.2970430-01 (789)	-398.280730
8.000	-975.375420	8.9527339-02	-975.285900	8.1863232-02 (789)	-398.280700
9.000	-975.375420	1.1824801-01	-975.257180	1.0441367-01 (789)	-398.280700
10.000	-975.433920	7.0694096-02	-975.363220	5.5570135-02 (789)	-398.280640
11.000	-975.433920	9.2122139-02	-975.341800	7.8082283-02 (789)	-398.280640
12.000	-975.468460	6.0007679-02	-975.408460	5.4717644-02 (789)	-398.280620
13.000	-975.468460	7.4590959-02	-975.393880	6.5881707-02 (789)	-398.280620
14.000	-975.496860	5.0434925-02	-975.446430	4.0495154-02 (789)	-398.280560
13.001,	-975.496860	6.1497940-02	-975.435360	5.2419754-02 (789)	-398.280560
15.000	-975.515570	4.3770200-02	-975.471800	3.9658034-02 (789)	-398.280460
17.000	-975.515570	5.1934335-02	-975.463040	4.5816085-02 (789)	-398.280460
18.000	-975.531430	3.7961078-02	-975.493470	3.0996983-02 (789)	-398.280360
19.000	-975.531430	4.4439885-02	-975.486490	3.8045207-02 (789)	-398.280360
20.000	-975.542810	3.3526919-02	-975.509290	3.0205399-02 (789)	-398.280260
21.000	-975.542810	3.8609313-02	-975.504200	3.4011597-02 (789)	-398.280260
22.000	-975.552470	2.9673229-02	-975.522790	2.4543335-02 (789)	-398.280120
23.000	-975.552470	3.3856199-02	-975.518610	2.9084059-02 (789)	-398.280120
24.000	-975.560090	2.6566579-02	-975.533520	2.3813953-02 (789)	-398.280020
25.000	-975.560090	2.9990373-02	-975.530100	2.6382446-02 (789)	-398.280020
26.000	-975.566600	2.3849235-02	-975.542750	1.9920524-02 (789)	-398.279860
27.000	-975.566600	2.6744547-02	-975.539860	2.3037360-02 (789)	-398.279860
28.000	-975.571880	2.1577938-02	-975.550300	1.9257906-02 (789)	-398.279740
29.000	-975.571880	2.4020132-02	-975.547860	2.1104624-02 (789)	-398.279740
30.000	-975.576410	1.9574450-02	-975.556840	1.6474465-02 (789)	-398.279610
31.000	-975.576410	2.1601925-02	-975.554730	1.8717112-02 (789)	-398.279610

RUN TERMINATED BECAUSE TOTAL ENERGY CHANGE IS LESS THAN 5.00000-06. DELPOT = 4.64532-06

ON THE LAST TIME STEP THE AVERAGE POTENTIAL ENERGY PER ATOM IS: -1.2364720+00, AND THE TOTAL NUMBER OF ATOMS IS: 789

THE AVERAGE POTENTIAL ENERGY PER MOVABLE ATOM IS: -1.3615490+00, AND THE NUMBER OF MOVABLE ATOMS IS: 424

CONFIGURATION ENERGY = -1.8917999+00

CRYSTAL AFTER RELAXATION: (100) ORIENTATION OF (X,Y) PLANES

(MOVABLE ATOMS ARE NOTED BY A TAG OF 0; IMMOVABLE ATOMS BY A TAG OF 1)

ATOM	X	Y	Z	P.ENERGY	TAG	TYPE	ATOM	X	Y	P.ENERGY	TAG	TYPE	
1	1.000000	1.000000	1.000000	-.3752646	1	1	2	3.000000	1.000000	1.000000	-.625441	1	1
3	5.000000	1.000000	1.000000	-.6254411	1	1	4	7.000000	1.000000	1.000000	-.625441	1	1
5	2.000000	2.000000	1.000000	-1.0007052	1	1	6	4.000000	2.000000	1.000000	-1.000702	1	1
7	6.000000	2.000000	1.000000	-1.0006979	1	1	8	1.000000	3.000000	1.000000	-.625441	1	1
9	2.999995	2.999994	1.000000	-1.0006998	0	1	10	4.999990	2.999977	1.000000	-1.000691	0	1
11	7.000006	2.999954	1.000000	-1.0006843	0	1	12	2.000000	4.000000	1.000000	-1.000701	1	1
13	3.999978	3.999969	1.000000	-1.0006897	0	1	14	5.999973	3.999922	1.000000	-1.000689	0	1
15	1.000000	5.000000	1.000000	-.6254411	1	1	16	2.999971	4.999977	1.000000	-1.000686	0	1
17	4.999940	4.999909	1.000000	-1.0006797	0	1	18	6.999986	4.999694	1.000000	-1.000661	0	1
19	2.000000	6.000000	1.000000	-1.0006900	1	1	20	3.999885	5.999942	1.000000	-1.000688	0	1
21	5.999925	6.000005	1.000000	-1.0007887	0	1	22	1.000000	7.000000	1.000000	-.625441	1	1
23	2.999892	7.000000	1.000000	-1.0006638	0	1	24	4.999498	7.000004	1.000000	-1.000665	0	1
25	6.999861	7.000139	1.000000	-1.0011990	0	1	26	2.000000	8.000000	1.000000	-1.000690	1	1
27	3.999880	8.000054	1.000000	-1.0006833	0	1	28	5.999903	8.000096	1.000000	-1.000775	0	1
29	1.000000	9.000000	1.000000	-.6254411	1	1	30	2.999969	9.000022	1.000000	-1.0006190	0	1
31	4.999895	9.000104	1.000000	-1.0006659	0	1	32	6.999996	9.000502	1.000000	-1.000666	0	1
33	2.000000	10.000000	1.000000	-1.0007012	1	1	34	3.999965	10.000035	1.000000	-1.000685	0	1
35	5.999946	10.000121	1.000000	-1.0006845	0	1	36	1.000000	11.000000	1.000000	-.625441	1	1
37	2.999993	11.000007	1.000000	-1.0006990	0	1	38	4.999979	11.000035	1.000000	-1.000688	0	1
39	7.000000	11.000115	1.000000	-1.0006680	0	1	40	2.000000	12.000000	1.000000	-1.000705	1	1
41	3.999995	12.000007	1.000000	-1.0007002	0	1	42	5.999990	12.000029	1.000000	-1.000691	0	1
43	1.000000	13.000000	1.000000	-.6254411	1	1	44	2.999999	13.000001	1.000000	-1.000704	0	1
45	4.999998	13.000005	1.000000	-1.0007019	0	1	46	7.000000	13.000004	1.000000	-1.000702	0	1
47	2.000000	14.000000	1.000000	-1.0007057	1	1	48	4.000000	14.000000	1.000000	-1.000705	1	1
49	6.000000	14.000000	1.000000	-1.0007048	1	1	50	1.000000	15.000000	1.000000	-.375265	1	1
51	3.000000	15.000000	1.000000	-.6254411	1	1	52	5.000000	15.000000	1.000000	-.625441	1	1
53	7.000000	15.000000	1.000000	-.6254411	1	1	54	2.000000	1.000000	2.000000	-1.000706	1	1
55	4.000000	1.000000	2.000000	-1.0007057	1	1	56	6.000000	1.000000	2.000000	-1.000706	1	1
57	1.000000	2.000000	2.000000	-1.0007057	1	1	58	3.000000	2.000000	2.000000	-1.501052	1	1
59	5.000000	2.000000	2.000000	-1.5010414	1	1	60	7.000000	2.000000	2.000000	-1.501046	1	1
61	2.000000	3.000000	2.000000	-1.5010519	1	1	62	3.999968	2.999953	2.000000	-1.501022	0	1
63	5.999971	2.999976	2.000000	-1.5009906	0	1	64	1.000000	4.000000	2.000000	-1.000706	1	1
65	2.999947	3.999947	2.000000	-1.5010147	0	1	66	4.999885	3.999802	2.000000	-1.500952	0	1
67	7.000041	3.999914	2.000000	-1.5009464	0	1	68	2.000000	5.000000	2.000000	-1.501020	1	1
69	3.999772	4.999793	2.000000	-1.5009298	0	1	70	5.999607	4.999654	2.000000	-1.500904	0	1
71	1.000000	6.000000	2.000000	-1.0007057	1	1	72	2.999774	5.999912	2.000000	-1.500947	0	1
73	4.999517	5.999571	2.000000	-1.5008667	0	1	74	6.999833	5.997895	2.000000	-1.500340	0	1
75	2.000000	7.000000	2.000000	-1.5010362	1	1	76	3.999081	6.999999	2.000000	-1.500732	0	1
77	5.997029	7.000209	2.000000	-1.5001724	0	1	78	1.000000	8.000000	2.000000	-1.000706	1	1
79	2.999785	8.000047	2.000000	-1.5009518	0	1	80	4.999474	8.000645	2.000000	-1.500852	0	1
81	6.999791	8.0002971	2.000000	-1.5001724	0	1	82	2.000000	9.000000	2.000000	-1.501031	1	1
83	3.999751	9.000197	2.000000	-1.5009229	0	1	84	5.999355	9.000525	2.000000	-1.500852	0	1

85	1.000000	10.000000	2.000000	-1.0007057	1	1	96	2.999943	10.000050	2.000000	-1.501014	0	1
87	4.999803	10.000250	2.000000	-1.5000236	0	1	98	7.000000	10.000020	2.000000	-1.500735	0	1
89	2.000000	11.000000	2.000000	-1.5010512	1	1	90	3.999950	11.000062	2.000000	-1.501016	0	1
91	5.999911	11.000226	2.000000	-1.5000459	0	1	92	1.000000	12.000000	2.000000	-1.000706	1	1
93	2.999991	12.000011	2.000000	-1.5010486	0	1	94	4.999975	12.000047	2.000000	-1.501032	0	1
95	6.999999	12.000037	2.000000	-1.5010364	0	1	96	2.000000	13.000000	2.000000	-1.501057	1	1
97	3.999996	13.000007	2.000000	-1.5010519	0	1	98	5.999999	13.000007	2.000000	-1.501052	0	1
99	1.000000	14.000000	2.000000	-1.0007057	1	1	100	3.000000	14.000000	2.000000	-1.501058	1	1
101	5.000000	14.000000	2.000000	-1.5010571	1	1	102	7.000000	14.000000	2.000000	-1.501057	1	1
103	2.000000	15.000000	2.000000	-1.0007057	1	1	104	4.000000	15.000000	2.000000	-1.000706	1	1
105	6.000000	15.000000	2.000000	-1.0007057	1	1	106	1.000000	1.000000	3.000000	-1.625441	1	1
107	3.000000	1.000000	3.000000	-1.0007057	1	1	108	5.000000	1.000000	3.000000	-1.000706	1	1
109	7.000000	1.000000	3.000000	-1.0007057	1	1	110	2.000000	2.000000	3.000000	-1.501055	1	1
111	4.000000	2.000000	3.000000	-1.5010395	1	1	112	6.000000	2.000000	3.000000	-1.501042	1	1
113	1.000000	3.000000	3.000000	-1.0007057	1	1	114	2.999961	2.999954	2.999981	-1.501021	0	1
115	4.999909	2.999944	2.999960	-1.5009699	0	1	116	7.000012	2.999900	3.000021	-1.501003	0	1
117	2.000000	4.000000	3.000000	-1.5010288	1	1	118	3.999807	3.999777	2.999886	-1.500933	0	1
119	5.999662	3.999314	2.999741	-1.5007892	0	1	120	1.000000	5.000000	3.000000	-1.000706	1	1
121	2.999747	4.999819	2.999943	-1.5009274	0	1	122	4.999436	4.999348	2.999464	-1.500782	0	1
123	6.999891	4.997190	2.998147	-1.5001826	0	1	124	2.000000	6.000000	3.000000	-1.501031	1	1
125	3.998946	5.999377	2.999625	-1.5007000	0	1	126	5.999392	5.999617	3.000608	-1.501782	0	1
127	1.000000	7.000000	3.000000	-1.0007057	1	1	128	2.999816	7.000004	3.000058	-1.500960	0	1
129	4.995660	6.999957	2.997072	-1.4993863	0	1	130	6.998102	7.001898	2.974274	-1.650337	0	1
131	2.000000	8.000000	3.000000	-1.5010324	1	1	132	3.999009	8.000583	2.999684	-1.500715	0	1
133	5.999005	8.000945	3.000997	-1.5017774	0	1	134	1.000000	9.000000	3.000000	-1.000706	1	1
135	2.999772	9.000165	2.999962	-1.5009382	0	1	136	4.999263	9.000737	2.999517	-1.500743	0	1
137	7.000043	9.000434	2.997072	-1.4993873	0	1	138	2.000000	10.000000	3.000000	-1.501032	1	1
139	3.999766	10.000235	2.999896	-1.5009232	0	1	140	5.999416	10.000492	2.999684	-1.500716	0	1
141	1.000000	11.000000	3.000000	-1.0007057	1	1	142	2.999954	11.000050	2.999983	-1.501020	0	1
143	4.999833	11.000239	2.999961	-1.5009468	0	1	144	6.999996	11.000195	3.000059	-1.500977	0	1
145	2.000000	12.000000	3.000000	-1.5010533	1	1	146	3.999967	12.000045	2.999994	-1.501030	0	1
147	5.999989	12.000044	3.000009	-1.5010335	0	1	148	1.000000	13.000000	3.000000	-1.000706	1	1
149	2.999995	13.000006	2.999999	-1.5010526	0	1	150	4.999997	13.000008	3.000001	-1.501052	0	1
151	7.000000	13.000009	3.000000	-1.5010505	0	1	152	2.000000	14.000000	3.000000	-1.501058	1	1
153	4.000000	14.000000	3.000000	-1.5010574	1	1	154	6.000000	14.000000	3.000000	-1.501057	1	1
155	1.000000	15.000000	3.000000	-1.6254411	1	1	156	3.000000	15.000000	3.000000	-1.000706	1	1
157	5.000000	15.000000	3.000000	-1.0007057	1	1	158	7.000000	15.000000	3.000000	-1.000706	1	1
159	2.000000	1.000000	4.000000	-1.0007057	1	1	160	4.000000	1.000000	4.000000	-1.000706	1	1
161	6.000000	1.000000	4.000000	-1.0007057	1	1	162	1.000000	2.000000	4.000000	-1.000706	1	1
163	3.000000	2.000000	4.000000	-1.5010445	1	1	164	5.000000	2.000000	4.000000	-1.501041	1	1
165	7.000000	2.000000	4.000000	-1.5010417	1	1	166	2.000000	3.000000	4.000000	-1.501039	1	1
167	3.999867	2.999865	3.999997	-1.5009773	0	1	168	5.999964	2.999912	3.999965	-1.501011	0	1
169	1.000000	4.000000	4.000000	-1.0007057	1	1	170	2.999811	3.999797	4.000000	-1.500952	0	1
171	4.999261	3.999271	3.999987	-1.5007496	0	1	172	6.999965	3.999777	3.999983	-1.501053	0	1
173	2.000000	5.000000	4.000000	-1.5010335	1	1	174	3.999047	4.999009	3.999995	-1.500702	0	1
175	5.996927	4.996062	4.000128	-1.5000660	0	1	176	1.000000	6.000000	4.000000	-1.000706	1	1
177	2.999872	5.999933	4.000003	-1.5000954	0	1	178	4.995748	5.996474	3.999899	-1.499512	0	1
179	6.998075	5.973904	4.001877	-1.6530159	0	1	180	2.000000	7.000000	4.000000	-1.501032	1	1
181	3.999032	6.999982	3.999962	-1.5010436	0	1	182	5.975657	6.999031	3.999520	-1.669651	0	1

183	1.000000	8.000000	4.000000	-1.0007057	1	1	184	2.999882	8.000062	4.000009	-1.500999	0	1
185	4.996045	8.003203	3.999977	-1.4995925	0	1	186	7.000369	8.024343	3.999520	-1.669650	0	1
187	2.000000	9.000000	4.000000	-1.5010355	1	1	188	3.999172	9.000875	4.000047	-1.500733	0	1
189	5.996797	9.003955	3.999977	-1.4995930	0	1	190	1.000000	10.000000	4.000000	-1.000706	1	1
191	2.999840	10.000174	4.000010	-1.5009658	0	1	192	4.999125	10.000830	4.000047	-1.500735	0	1
193	7.000018	10.000369	3.999962	-1.5010462	0	1	194	2.000000	11.000000	4.000000	-1.501042	1	1
195	3.999825	11.000170	4.000010	-1.5009718	0	1	196	5.999937	11.000128	4.000009	-1.501005	0	1
197	1.000000	12.000000	4.000000	-1.0007057	1	1	198	2.999973	12.000027	4.000001	-1.501039	0	1
199	4.999982	12.000037	4.000002	-1.5010362	0	1	200	6.999999	12.000047	4.000003	-1.501032	0	1
201	2.000000	13.000000	4.000000	-1.5010557	1	1	202	3.999997	13.000007	4.000000	-1.501053	0	1
203	5.999998	13.000010	4.000000	-1.5010500	0	1	204	1.000000	14.000000	4.000000	-1.000706	1	1
205	3.000000	14.000000	4.000000	-1.5010576	1	1	206	5.000000	14.000000	4.000000	-1.501057	1	1
207	7.000000	14.000000	4.000000	-1.5010569	1	1	208	2.000000	15.000000	4.000000	-1.000706	1	1
209	4.000000	15.000000	4.000000	-1.0007057	1	1	210	6.000000	15.000000	4.000000	-1.000706	1	1
211	1.000000	1.000000	5.000000	-1.6254411	1	1	212	3.000000	1.000000	5.000000	-1.000706	1	1
213	5.000000	1.000000	5.000000	-1.0007057	1	1	214	7.000000	1.000000	5.000000	-1.000706	1	1
215	2.000000	2.000000	5.000000	-1.5010550	1	1	216	4.000000	2.000000	5.000000	-1.501037	1	1
217	6.000000	2.000000	5.000000	-1.5010405	1	1	218	1.000000	3.000000	5.000000	-1.000706	1	1
219	2.999960	2.999953	5.000018	-1.5010197	0	1	220	4.999883	2.999817	5.000031	-1.500957	0	1
221	7.000010	2.999878	4.999953	-1.5009954	0	1	222	2.000000	4.000000	5.000000	-1.501029	1	1
223	3.999768	3.999770	5.000107	-1.5009277	0	1	224	5.999539	3.999167	5.000260	-1.500735	0	1
225	1.000000	5.000000	5.000000	-1.0007057	1	1	226	2.999760	4.999834	5.000058	-1.500933	0	1
227	4.999359	4.999340	5.000510	-1.5007594	0	1	228	6.999792	4.996444	5.002377	-1.499954	0	1
229	2.000000	6.000000	5.000000	-1.5010328	1	1	230	3.999007	5.999444	5.000333	-1.500721	0	1
231	5.998878	5.999851	4.999681	-1.5017478	0	1	232	1.000000	7.000000	5.000000	-1.000706	1	1
233	2.999837	7.000006	4.999949	-1.5009778	0	1	234	4.995888	7.000057	5.002529	-1.499501	0	1
235	7.000349	6.999651	5.002909	-1.6090855	0	1	236	2.000000	8.000000	5.000000	-1.501034	1	1
237	3.999075	8.000541	5.000339	-1.5007298	0	1	238	6.000346	7.999654	4.998345	-1.502123	0	1
239	1.000000	9.000000	5.000000	-1.0007057	1	1	240	2.999782	9.000152	5.000054	-1.500941	0	1
241	4.999689	9.000311	5.000494	-1.5008664	0	1	242	6.999943	9.000413	5.002529	-1.499502	0	1
243	2.000000	10.000000	5.000000	-1.5010326	1	1	244	3.999855	10.000146	5.000127	-1.500957	0	1
245	5.999458	10.000927	5.000339	-1.5007319	0	1	246	1.000000	11.000000	5.000000	-1.000706	1	1
247	2.999967	11.000036	5.000020	-1.5010276	0	1	248	4.999845	11.000228	5.000055	-1.500948	0	1
249	6.999994	11.000173	4.999948	-1.5009844	0	1	250	2.000000	12.000000	5.000000	-1.501055	1	1
251	3.999969	12.000043	5.000008	-1.5010321	0	1	252	5.999991	12.000042	4.999995	-1.501033	0	1
253	1.000000	13.000000	5.000000	-1.0007057	1	1	254	2.999996	13.000006	5.000001	-1.501053	0	1
255	4.999998	13.000000	5.000000	-1.5010512	0	1	256	7.000000	13.000000	5.000001	-1.501051	0	1
257	2.000000	14.000000	5.000000	-1.5010581	1	1	258	4.000000	14.000000	5.000000	-1.501057	1	1
259	6.000000	14.000000	5.000000	-1.5010571	1	1	260	1.000000	15.000000	5.000000	-1.625441	1	1
261	3.000000	15.000000	5.000000	-1.0007057	1	1	262	5.000000	15.000000	5.000000	-1.000706	1	1
263	7.000000	15.000000	5.000000	-1.0007057	1	1	264	2.000000	1.000000	6.000000	-1.000706	1	1
265	4.000000	1.000000	6.000000	-1.0007057	1	1	266	6.000000	1.000000	6.000000	-1.000706	1	1
267	1.000000	2.000000	6.000000	-1.0007057	1	1	268	3.000000	2.000000	6.000000	-1.501051	1	1
269	5.000000	2.000000	6.000000	-1.5010371	1	1	270	7.000000	2.000000	6.000000	-1.501044	1	1
271	2.000000	3.000000	6.000000	-1.5010514	1	1	272	3.999957	2.999943	6.000000	-1.501016	0	1
273	5.999945	2.999937	6.000000	-1.5009716	0	1	274	1.000000	4.000000	6.000000	-1.000706	1	1
275	2.999944	3.999945	6.000000	-1.5010130	0	1	276	4.999822	3.999754	6.000000	-1.500928	0	1
277	7.000002	3.999295	6.000000	-1.5007744	0	1	278	2.000000	5.000000	6.000000	-1.501031	1	1
279	3.999752	4.999778	6.000000	-1.5009241	0	1	280	5.999346	4.999487	6.000000	-1.500956	0	1

281	1.000000	6.000000	6.000000	-1.0007057	1	1
283	4.999379	5.999402	6.000000	-1.5008421	0	1
285	2.000000	7.000000	6.000000	-1.5010383	1	1
287	5.996984	7.000000	6.000000	-1.4996741	0	1
289	2.999804	8.000078	6.000000	-1.5009594	0	1
291	6.999995	8.003016	6.000000	-1.4996746	0	1
293	3.999833	9.000148	6.000000	-1.5009549	0	1
295	1.000000	10.000000	6.000000	-1.0007057	1	1
297	4.999852	10.000168	6.000000	-1.5009558	0	1
299	2.000000	11.000000	6.000000	-1.5010529	1	1
301	5.999920	11.000206	6.000000	-1.5009663	0	1
303	2.999993	12.000008	6.000000	-1.5010500	0	1
305	6.999999	12.000034	6.000000	-1.5010383	0	1
307	3.999996	13.000007	6.000000	-1.5010524	0	1
309	1.000000	14.000000	6.000000	-1.0007057	1	1
311	5.000000	14.000000	6.000000	-1.5010576	1	1
313	2.000000	15.000000	6.000000	-1.0007057	1	1
315	6.000000	15.000000	6.000000	-1.0007057	1	1
317	3.000000	1.000000	7.000000	-.6254411	1	1
319	7.000000	1.000000	7.000000	-.6254411	1	1
321	4.000000	2.000000	7.000000	-1.0007005	1	1
323	1.000000	3.000000	7.000000	-.6254411	1	1
325	4.999978	2.999964	7.000000	-1.0006845	0	1
327	2.000000	4.000000	7.000000	-1.0007010	1	1
329	5.999929	3.999866	7.000000	-1.0006742	0	1
331	2.999966	4.999975	7.000000	-1.0006850	0	1
333	7.000001	4.999420	7.000000	-1.0006478	0	1
335	3.999857	5.999938	7.000000	-1.0006776	0	1
337	1.000000	7.000000	7.000000	-.6254411	1	1
339	4.999481	6.999988	7.000000	-1.0006542	0	1
341	2.000000	8.000000	7.000000	-1.0006926	1	1
343	6.000009	7.999991	7.000000	-1.0007868	0	1
345	2.999976	9.000019	7.000000	-1.0006895	0	1
347	7.000012	9.000519	7.000000	-1.0006404	0	1
349	3.999973	10.000027	7.000000	-1.0006893	0	1
351	1.000000	11.000000	7.000000	-.6254411	1	1
353	4.999981	11.000028	7.000000	-1.0006926	0	1
355	2.000000	12.000000	7.000000	-1.0007045	1	1
357	5.999991	12.000025	7.000000	-1.0006931	0	1
359	2.999999	13.000000	7.000000	-1.0007041	0	1
361	7.000000	13.000004	7.000000	-1.0007017	0	1
363	4.000000	14.000000	7.000000	-1.0007045	1	1
365	1.000000	15.000000	7.000000	-.3752646	1	1
367	5.000000	15.000000	7.000000	-.6254411	1	1
369	9.000000	1.000000	1.000000	-.6254411	1	1
371	13.000000	1.000000	1.000000	-.6254411	1	1
373	8.000000	2.000000	1.000000	-1.0006988	1	1
375	12.000000	2.000000	1.000000	-1.0007050	1	1
377	9.000000	2.999994	1.000000	-1.0007000	0	1

282	2.999797	5.999930	6.000000	-1.500958	0	1
284	7.000037	5.996651	6.000000	-1.499572	0	1
286	3.999197	7.000038	6.000000	-1.500764	0	1
288	1.000000	8.000000	6.000000	-1.000706	1	1
290	4.999785	8.000540	6.000000	-1.500935	0	1
292	2.000000	9.000000	6.000000	-1.501033	1	1
294	5.999460	9.000215	6.000000	-1.500935	0	1
296	2.999957	10.000039	6.000000	-1.501022	0	1
298	6.999962	10.000804	6.000000	-1.500765	0	1
300	3.999961	11.000047	6.000000	-1.501024	0	1
302	1.000000	12.000000	6.000000	-1.000706	1	1
304	4.999978	12.000044	6.000000	-1.501033	0	1
306	2.000000	13.000000	6.000000	-1.501058	1	1
308	5.999999	13.000006	6.000000	-1.501053	0	1
310	3.000000	14.000000	6.000000	-1.501057	1	1
312	7.000000	14.000000	6.000000	-1.501057	1	1
314	4.000000	15.000000	6.000000	-1.000706	1	1
316	1.000000	1.000000	7.000000	-.375265	1	1
318	5.000000	1.000000	7.000000	-.625441	1	1
320	2.000000	2.000000	7.000000	-1.000705	1	1
322	6.000000	2.000000	7.000000	-1.000695	1	1
324	2.999993	2.999993	7.000000	-1.000698	0	1
326	7.000000	2.999924	7.000000	-1.000672	0	1
328	3.999968	3.999963	7.000000	-1.000685	0	1
330	1.000000	5.000000	7.000000	-.625441	1	1
332	4.999899	4.999903	7.000000	-1.000671	0	1
334	2.000000	6.000000	7.000000	-1.000692	1	1
336	5.999953	5.999941	7.000000	-1.000820	0	1
338	2.999909	7.000005	7.000000	-1.000669	0	1
340	7.000087	6.999913	7.000000	-1.001299	0	1
342	3.999911	8.000062	7.000000	-1.000691	0	1
344	1.000000	9.000000	7.000000	-.625441	1	1
346	4.999925	9.000075	7.000000	-1.000673	0	1
348	2.000000	10.000000	7.000000	-1.000702	1	1
350	5.999938	10.000089	7.000000	-1.000691	0	1
352	2.999994	11.000006	7.000000	-1.000700	0	1
354	6.999995	11.000006	7.000000	-1.000673	0	1
356	3.999996	12.000006	7.000000	-1.000701	0	1
358	1.000000	13.000000	7.000000	-.625441	1	1
360	4.999998	13.000005	7.000000	-1.000703	0	1
362	2.000000	14.000000	7.000000	-1.000705	1	1
364	6.000000	14.000000	7.000000	-1.000705	1	1
366	3.000000	15.000000	7.000000	-.625441	1	1
368	7.000000	15.000000	7.000000	-.625441	1	1
370	11.000000	1.000000	1.000000	-.625441	1	1
372	15.000000	1.000000	1.000000	-.375265	1	1
374	10.000000	2.000000	1.000000	-1.000704	1	1
376	14.000000	2.000000	1.000000	-1.000705	1	1
378	11.000001	2.999998	1.000000	-1.000703	0	1

379	13.000000	3.000000	1.000000	-1.0007045	0	1	380	15.000000	3.000000	1.000000	-1.625441	1	1
381	8.000031	3.999978	1.000000	-1.0007033	0	1	382	10.000008	3.999991	1.000000	-1.000698	0	1
383	12.000001	3.999999	1.000000	-1.0007036	0	1	384	14.000000	4.000000	1.000000	-1.000705	1	1
385	9.000026	4.999974	1.000000	-1.0006857	0	1	386	11.000007	4.999994	1.000000	-1.000701	0	1
387	13.000002	4.999999	1.000000	-1.0007036	0	1	388	15.000000	5.000000	1.000000	-1.625441	1	1
389	7.999942	6.000058	1.000000	-1.0007541	0	1	390	10.000022	5.999969	1.000000	-1.000703	0	1
391	12.000011	5.999996	1.000000	-1.0006986	0	1	392	14.000000	6.000000	1.000000	-1.000705	1	1
393	9.000305	7.000014	1.000000	-1.0006607	0	1	394	11.000048	6.999994	1.000000	-1.000687	0	1
395	13.000002	7.000000	1.000000	-1.0007033	0	1	396	15.000000	7.000000	1.000000	-1.625441	1	1
397	7.999995	8.000005	1.000000	-1.0007885	0	1	398	10.000078	8.000026	1.000000	-1.000689	0	1
399	12.000013	8.000002	1.000000	-1.0006974	0	1	400	14.000000	8.000000	1.000000	-1.000705	1	1
401	9.000091	9.000009	1.000000	-1.0006795	0	1	402	11.000025	9.000010	1.000000	-1.000693	0	1
403	13.000002	9.000001	1.000000	-1.0007038	0	1	404	15.000000	9.000000	1.000000	-1.625441	1	1
405	8.000057	10.000116	1.000000	-1.0006876	0	1	406	10.000031	10.000022	1.000000	-1.000690	0	1
407	12.000005	10.000002	1.000000	-1.0007017	0	1	408	14.000000	10.000000	1.000000	-1.000705	1	1
409	9.000022	11.000033	1.000000	-1.0006900	0	1	410	11.000006	11.000005	1.000000	-1.000701	0	1
411	13.000000	11.000000	1.000000	-1.0007038	0	1	412	15.000000	11.000000	1.000000	-1.625441	1	1
413	8.000010	12.000030	1.000000	-1.0006907	0	1	414	10.000005	12.000007	1.000000	-1.000701	0	1
415	12.000001	12.000000	1.000000	-1.0007038	0	1	416	14.000000	12.000000	1.000000	-1.000705	1	1
417	9.000002	13.000005	1.000000	-1.0007017	0	1	418	11.000001	13.000001	1.000000	-1.000704	0	1
419	13.000000	13.000000	1.000000	-1.0007050	0	1	420	15.000000	13.000000	1.000000	-1.625441	1	1
421	8.000000	14.000000	1.000000	-1.0007050	1	1	422	10.000000	14.000000	1.000000	-1.000705	1	1
423	12.000000	14.000000	1.000000	-1.0007055	1	1	424	14.000000	14.000000	1.000000	-1.000706	1	1
425	9.000000	15.000000	1.000000	-1.6254411	1	1	426	11.000000	15.000000	1.000000	-1.625441	1	1
427	13.000000	15.000000	1.000000	-1.6254411	1	1	428	15.000000	15.000000	1.000000	-1.375265	1	1
429	8.000000	1.000000	2.000000	-1.0007057	1	1	430	10.000000	1.000000	2.000000	-1.000706	1	1
431	12.000000	1.000000	2.000000	-1.0007057	1	1	432	14.000000	1.000000	2.000000	-1.000706	1	1
433	9.000000	2.000000	2.000000	-1.5010450	1	1	434	11.000000	2.000000	2.000000	-1.501057	1	1
435	13.000000	2.000000	2.000000	-1.5010579	1	1	436	15.000000	2.000000	2.000000	-1.000706	1	1
437	8.000045	2.999989	2.000000	-1.5009985	0	1	438	10.000013	2.999987	2.000000	-1.501043	0	1
439	12.000002	2.999998	2.000000	-1.5010545	0	1	440	14.000000	3.000000	2.000000	-1.501058	1	1
441	9.000055	3.999951	2.000000	-1.5010107	0	1	442	11.000014	3.999987	2.000000	-1.501043	0	1
443	13.000003	3.999998	2.000000	-1.5010552	0	1	444	15.000000	4.000000	2.000000	-1.000706	1	1
445	8.000301	5.000078	2.000000	-1.5010169	0	1	446	10.000050	4.999945	2.000000	-1.501011	0	1
447	12.000020	4.999989	2.000000	-1.5010450	0	1	448	14.000000	5.000000	2.000000	-1.501058	1	1
449	8.999922	5.999968	2.000000	-1.5010173	0	1	450	11.000109	5.999954	2.000000	-1.501003	0	1
451	13.000003	5.999999	2.000000	-1.5010550	0	1	452	15.000000	6.000000	2.000000	-1.000706	1	1
453	8.002105	7.000167	2.000000	-1.5003400	0	1	454	10.000486	6.999959	2.000000	-1.500847	0	1
455	12.000016	6.999997	2.000000	-1.5010459	0	1	456	14.000000	7.000000	2.000000	-1.501058	1	1
457	9.000346	8.000393	2.000000	-1.5009046	0	1	458	11.000128	8.000030	2.000000	-1.500995	0	1
459	13.000003	8.000000	2.000000	-1.5010545	0	1	460	15.000000	8.000000	2.000000	-1.000706	1	1
463	12.000026	9.000483	2.000000	-1.5008671	0	1	462	10.000198	9.000115	2.000000	-1.500952	0	1
			2.000000	-1.5010409	0	1	464	14.000000	9.000000	2.000000	-1.501058	1	1
465	9.000206	10.000229	2.000000	-1.5009303	0	1	466	11.000050	10.000031	2.000000	-1.501025	0	1
467	13.000004	10.000001	2.000000	-1.5010545	0	1	468	15.000000	10.000000	2.000000	-1.000706	1	1
469	8.000091	11.000238	2.000000	-1.5009558	0	1	470	10.000052	11.000057	2.000000	-1.501018	0	1
471	12.000008	11.000005	2.000000	-1.5010514	0	1	472	14.000000	11.000000	2.000000	-1.501058	1	1
473	9.000026	12.000051	2.000000	-1.5010293	0	1	474	11.000609	12.000010	2.000000	-1.501050	0	1
475	13.000001	12.000000	2.000000	-1.5010560	0	1	476	15.000000	12.000000	2.000000	-1.000706	1	1

477	8.000001	13.000007	2.000000	-1.5010526	0	1	478	10.000004	13.000008	2.000000	-1.501052	0	1
479	12.000001	13.000001	2.000000	-1.5010562	0	1	480	14.000000	13.000000	2.000000	-1.501050	1	1
481	9.000000	14.000000	2.000000	-1.5010574	1	1	482	11.000000	14.000000	2.000000	-1.501057	1	1
483	13.000000	14.000000	2.000000	-1.5010586	1	1	484	15.000000	14.000000	2.000000	-1.000706	1	1
485	8.000000	15.000000	2.000000	-1.0007057	1	1	486	10.000000	15.000000	2.000000	-1.000706	1	1
487	12.000000	15.000000	2.000000	-1.0007057	1	1	488	14.000000	15.000000	2.000000	-1.000706	1	1
489	9.000000	1.000000	3.000000	-1.0007057	1	1	490	11.000000	1.000000	3.000000	-1.000706	1	1
491	13.000000	1.000000	3.000000	-1.0007057	1	1	492	15.000000	1.000000	3.000000	-.625441	1	1
493	8.000000	2.000000	3.000000	-1.5010433	1	1	494	10.000000	2.000000	3.000000	-1.501045	1	1
495	12.000000	2.000000	3.000000	-1.5010569	1	1	496	14.000000	2.000000	3.000000	-1.501050	1	1
497	9.000079	2.999985	2.999962	-1.5009894	0	1	498	11.000011	2.999990	2.999989	-1.501046	0	1
499	13.000002	2.999998	3.000000	-1.5010562	0	1	500	15.000000	3.000000	3.000000	-1.000706	1	1
501	8.000317	3.999457	2.999758	-1.5008314	0	1	502	10.000037	3.999963	2.999919	-1.501014	0	1
503	12.000019	3.999986	2.999995	-1.5010448	0	1	504	14.000000	4.000000	3.000000	-1.501058	1	1
505	8.999969	5.000031	2.999657	-1.5009866	0	1	506	11.000119	4.999920	2.999962	-1.500993	0	1
507	13.000004	4.999999	3.000000	-1.5010543	0	1	508	15.000000	5.000000	3.000000	-1.000706	1	1
509	7.998886	6.001114	3.001888	-1.5021214	0	1	510	10.000543	5.999683	2.999758	-1.500833	0	1
511	12.000023	5.999994	3.000001	-1.5010440	0	1	512	14.000000	6.000000	3.000000	-1.501058	1	1
513	9.0002810	7.000109	2.998147	-1.5001819	0	1	514	11.000105	6.999988	3.000022	-1.501007	0	1
515	13.000004	7.000000	2.999999	-1.5010543	0	1	516	15.000000	7.000000	3.000000	-1.000706	1	1
517	8.000382	8.000608	3.000608	-1.5017822	0	1	518	10.000681	8.000338	2.999741	-1.500791	0	1
519	12.000025	8.000001	3.000001	-1.5010424	0	1	520	14.000000	8.000000	3.000000	-1.501058	1	1
521	9.000651	9.000364	2.999464	-1.5007811	0	1	522	11.000162	9.000092	2.999959	-1.500974	0	1
523	13.000004	9.000001	3.000000	-1.5010538	0	1	524	15.000000	9.000000	3.000000	-1.000706	1	1
525	8.000623	10.001056	2.999625	-1.5007014	0	1	526	10.000223	10.000194	2.999886	-1.500934	0	1
527	12.000028	10.000017	2.999994	-1.5010386	0	1	528	14.000000	10.000000	3.000000	-1.501058	1	1
529	9.000184	11.000265	2.999943	-1.5009358	0	1	530	11.000048	11.000042	2.999983	-1.501025	0	1
531	13.000003	11.000002	2.999999	-1.5010545	0	1	532	15.000000	11.000000	3.000000	-1.000706	1	1
533	8.000009	12.000046	3.000009	-1.5010316	0	1	534	10.000037	12.000051	2.999991	-1.501027	0	1
535	12.000007	12.000006	2.999998	-1.5010519	0	1	536	14.000000	12.000000	3.000000	-1.501058	1	1
537	9.000002	13.000009	3.000001	-1.5010509	0	1	538	11.000005	13.000007	2.999999	-1.501052	0	1
539	13.000000	13.000000	3.000000	-1.5010567	0	1	540	15.000000	13.000000	3.000000	-1.000706	1	1
541	8.000000	14.000000	3.000000	-1.5010571	1	1	542	10.000000	14.000000	3.000000	-1.501057	1	1
543	12.000000	14.000000	3.000000	-1.5010576	1	1	544	14.000000	14.000000	3.000000	-1.501058	1	1
545	9.000000	15.000000	3.000000	-1.0007057	1	1	546	11.000000	15.000000	3.000000	-1.000706	1	1
547	13.000000	15.000000	3.000000	-1.0007057	1	1	548	15.000000	15.000000	3.000000	-.625441	1	1
549	8.000000	1.000000	4.000000	-1.0007057	1	1	550	10.000000	1.000000	4.000000	-1.000706	1	1
551	12.000000	1.000000	4.000000	-1.0007057	1	1	552	14.000000	1.000000	4.000000	-1.000706	1	1
553	9.000000	2.000000	4.000000	-1.5010455	1	1	554	11.000000	2.000000	4.000000	-1.501050	1	1
555	13.000000	2.000000	4.000000	-1.5010569	1	1	556	15.000000	2.000000	4.000000	-1.000706	1	1
557	8.000034	2.999931	3.999979	-1.5010202	0	1	558	10.000094	2.999914	3.999988	-1.501004	0	1
559	12.000012	2.999987	3.999999	-1.5010486	0	1	560	14.000000	3.000000	4.000000	-1.501058	1	1
561	9.000548	3.999492	3.999935	-1.5008254	0	1	562	11.000090	3.999906	3.999988	-1.501007	0	1
563	13.000003	3.999999	4.000000	-1.5010548	0	1	564	15.000000	4.000000	4.000000	-1.000706	1	1
565	8.002243	4.997234	4.000051	-1.5002258	0	1	566	10.000509	4.999452	3.999935	-1.500826	0	1
567	12.000019	4.999491	3.999997	-1.5010450	0	1	568	14.000000	5.000000	4.000000	-1.501058	1	1
569	9.002766	5.997757	4.000051	-1.5002265	0	1	570	11.000074	5.999966	3.999979	-1.501024	0	1
571	13.000004	5.999499	4.000000	-1.5010540	0	1	572	15.000000	6.000000	4.000000	-1.000706	1	1
573	8.026006	7.001925	4.001877	-1.6530163	0	1	574	10.000223	7.000035	3.999983	-1.501053	0	1

575	12.000027	6.999999	3.999996	-1.5010402	0	1
577	9.003338	8.003073	4.000128	-1.5009668	0	1
579	13.000005	8.000000	4.000000	-1.5010536	0	1
581	8.003526	9.004253	3.999899	-1.4995115	0	1
583	12.000025	9.000009	3.999997	-1.5010426	0	1
585	9.000991	10.000955	3.999995	-1.5007038	0	1
587	13.000004	10.000001	4.000000	-1.5010543	0	1
589	8.000067	11.000138	4.000003	-1.5010035	0	1
591	12.000021	11.000019	4.000000	-1.5010433	0	1
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