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A Computer Program for the Simulation of Solid Solutions

R. O. Williams

OAK RIDGE NATIONAL LABORATORY

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OF SOLID SOLUTIONS

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MAY 1976

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R. O. Williams

ABSTRACT

This report describes a computer program which rearranges the atoms on a lattice containing 12,075 sites until the populations in a set of 18 shells are in agreement with those calculated from x-ray measurements. To improve the accuracy, eight independent runs are made. Because of the large amount of computation involved, considerable effort went into selecting an efficient algorithm and constructing the program for the most efficient execution.

The output consists of a model showing the atoms that have been moved from their initial position; the output also gives shell populations (including error estimates). Also, the intensity is calculated for both the x-ray data and the model. Finally, various structural features for the model are determined and compared with the same features in the initial random model.

The program is written for the face-centered cubic lattice, but its conversion for modeling the body-centered cubic lattice would not be difficult.

INTRODUCTION

One of the very interesting aspects of metallic solid solutions is that, in general, the atoms are not randomly arranged on the lattice. If the solution has a positive heat of mixing, like atoms cluster together, and ultimately, at a sufficiently low temperature, actual phase separation may take place within the miscibility gap. Alternately, if the heat of mixing is negative, then generally there is a preference for unlike first neighbors. A negative heat of mixing is generally observed to occur in systems in which new phases or ordered regions are found, and the usual observation is that the short-range order in the solution is similar to that in the ordered phase, provided the two lattices are similar.

The presence of this nonrandomness is of considerable importance in understanding such solutions. In particular, the nonrandomness is a function of temperature, thus giving an extra contribution to the specific heat and, therefore, a temperature-dependent heat of mixing and entropy. Further, the presence of this nonrandomness is recognized as one source

of solid-solution strengthening. When such materials are annealed for long times at temperatures where the atomic mobility is low, there can be long-time changes in the solids which complicate their application or lead to questions of interpretation of experimental observations.

The most advanced technique for quantitatively studying such solutions is by measurements of the diffuse scattering of x rays. It can be shown that if the atoms sit precisely on the lattice sites, then all the diffuse scattering can be described in terms of a set of conditional probabilities, the so-called alphas due to Cowley and Warren. Thus it follows that the only information which can be obtained from such measurements is the value of each alpha. Deviations in the position of the atoms from the perfect lattice give rise to additional features in the diffuse scattering which are interesting but are not of concern in this report.

Having obtained a set of alphas, one wants to arrive at certain conclusions about the nature of the solution. For example, copper-gold alloys around the composition Cu_3Au exhibit diffuse scattering which has broad peaks at the superlattice positions for the ordered structure. Of concern is the extent to which it is proper to consider the short-range order structure as having long-range order with a very small domain size. Constructing a model which reproduces the observations and from which such conclusions can be examined proves to be a rather difficult task, primarily because the model needs to contain a large number of atoms.

The approach of Gehlen and Cohen¹ to this problem was to interchange atoms in a large model, using a computer, until the populations in the first few shells were in agreement with the observations. (The nearest neighbors of an atom are collectively called the first shell, and similarly, the more distant atoms are arranged in higher-order shells.) The author had developed a similar program,² and our experience over the years has shown that a fairly large number of shells must be matched to get adequate agreement.³ Also, the original size of 8000 sites was not sufficiently large for statistical reasons, and further, there are many things which may be done with the model which help in understanding its structure. In particular, in deciding if a model is really an adequate representation of the observations, we have found it very helpful to calculate the x-ray intensity given by the model.³

¹P. C. Gehlen and J. B. Cohen, "Computer Simulation of the Structure Associated with Local Order in Alloys," *Phys. Rev.* 139: A844-55 (1965).

²R. O. Williams, *A Computer Program for the Simulation of Solid Solutions from X-Ray Data*, ORNL-TM-2866 (1970).

³R. O. Williams, "Short Range Order Structure in a Copper 16 Atomic Percent Aluminum Alloy," *Metall. Trans.* 5: 1843-50 (1974).

This report is the documentation of a new, expanded program. It initially describes the mathematical basis of the algorithm, then gives the basic steps in carrying out the solution, and concludes with an analysis of the process.

THEORY

The diffuse intensity (in units of the Laue monotonic intensity) is given as

$$I = 1 + \sum_{i=1}^n \alpha_i \sum_{j=1}^M \cos \omega_j , \quad (1)$$

where the inner sum is over all M sites in the j th shell, and the outer sum is over all shells which have alphas significantly different from zero. The angle ω is given as

$$\omega = 2\pi (h_1 \ell + h_2 m + h_3 n) , \quad (2)$$

where h_1 , h_2 , and h_3 are the components of the reciprocal lattice vector, and ℓ , m , and n are the coordinates of the atoms in the shell. Representing the two kinds of atoms as 0 and 1, the alphas are defined as

$$\alpha_i = 1 - \frac{P}{x_0} , \quad (3)$$

where P is the probability of finding a 0 atom in the i th shell of a 1 atom, and x_0 is the atom fraction of 0 atoms. In the absence of long-range order, the correlation approaches zero for shells of larger diameter such that P approaches x_0 , and the alphas approach zero. Thus the sums have a finite number of terms, and, as a matter of observation, solid solutions require no more than 50 alphas for their description.

The above definition of the intensity applies to a physical model as well as to a real material, and the degree of difference between the two, the variance, is defined as

$$V = \int_0^1 \int_0^1 \int_0^1 (I_1 - I_2)^2 dh_1 dh_2 dh_3 , \quad (4)$$

where the subscripts identify the observations and the model. Substituting into Eq. (1) and carrying out the integration leads to

$$V = \frac{1}{2} \sum_{i=1}^n M_i (\alpha_{i_1} - \alpha_{i_2})^2 \quad (5)$$

as a result of the orthogonality of the terms in the series; M_i is the number of sites in the i th shell. For a model containing L atoms, the number of 1 atoms in the i th shell around a 1 center atom is related to the alpha for that shell by the expression

$$N_i = (x_1 + \alpha_i x_0) M_i x_1 L / 2, \quad (6)$$

where the factor of 1/2 arises because we count each such pair only once, but it contributes twice to the particular shell, since either end can be the center atom. The variance between a given model and one which agrees with the set of observed alphas is now given as

$$V = \frac{2}{(x_1 x_0 L)^2} \sum_{i=1}^n \frac{(N_{i_1} - N_{i_2})^2}{M_i}. \quad (7)$$

We refer to these differences in the number of 1-1 pairs for the various shells as the components of our design vector. We take the length of the vector to be

$$W = \left[48 \sum_{i=1}^n \frac{(N_{i_1} - N_{i_2})^2}{M_i} \right]^{\frac{1}{2}} \quad (8)$$

such that the square of the length is proportional to the variance. Thus the minimization of the length of the vector minimizes the variance.

Consider now a pair of sites, one of each kind. Were these two atoms to be interchanged, the new length of our design vector would be

$$W = \left[48 \sum_{i=1}^n \frac{(N_{i_1} - N_{i_2} + N1 - N0)^2}{M_i} \right]^{\frac{1}{2}}, \quad (9)$$

where $N0$ is the number of 1 atoms in the i th shell around the 0 atom, and similarly, $N1$ is the number for the 1 atom. The subscript 1 represents the finished model, and 2 represents the present model. Thus if the new length is less, then the interchange is favorable. If the two

sites are close enough to be mutually in a shell included in the design set, then, for that shell, the improvement is numerically one less. This occurs rather infrequently and need not concern us here, but it must be taken care of in the program.

Thus the simplest strategy, that of interchanging favorable mixed pairs chosen at random, must lead to an improvement in the model, and this process can be continued, in theory, until either the vector is of zero length or no pair remains which can provide a reduction in length. A refined strategy, the one actually used in the program, is as follows. Instead of discarding both members when no favorable interchange is possible, we may examine a second 0 site and save that 0 site which gives the shortest vector. Assuming that the interchange is still unfavorable, we similarly compare a new 1 site to the first one and save the most favorable site. We continue this process of alternately examining 0 and 1 sites, always saving the new site if it is more favored, until we find a pair which is favorable for interchange. Further, the examination of the successive shells for a given site is abandoned whenever the vector length exceeds that of the previously chosen best pair in the string.

PROGRAM DOCUMENTATION

The basic model consists of a simple cubic lattice with edges of 21, 23, and 25 sites which contains 12,075 sites. This basic volume is translated along its edges to introduce periodic boundaries, thus eliminating free surfaces. The simple cubic lattice represents two interpenetrating fcc lattices, and, since we have an odd number of edge cells in the basic lattice, we transfer from one fcc lattice to the other at the periodic boundaries. The interested reader should have little difficulty in working out the precise repeat vectors for structure.

The basic program can be modified without difficulty to model a body-centered cubic lattice. For this case the basic lattice represents four interpenetrating bcc lattices which will have repeat vectors different from the fcc lattice.

In order to carry out the modeling without having to use translations to reflect the boundaries, the basic lattice is extended to $29 \times 31 \times 33$ for modeling, which limits the components of the shells in the design set to four. All 18 possible shells, which contain a total of 264 sites, are used. When shell counts are required for the alphas, the model is further extended to a $29 \times 39 \times 41$ volume, which limits the alphas to shells having components of eight or less. Going beyond these limits requires modifications to the size of the lattices.

The main program, MODEL, sets up the starting structure, carries out the scanning of the sites, tests for possible interchanges, calls the subroutines as required, and calculates the alphas. Subroutine EXCH

carries out the interchange and tests for completion of the modeling. Subroutine ADJUST adjusts secondary sites as required by the proximity of the boundaries. SHELL carries out the necessary counts and calculates the vector length. Subroutine SORT determines the numbers of various configurations in the model. Then DISY prints out the model. Subroutine ALPHA carries out the shell counts required to calculate the alphas in the finished model. The calculation of the intensity for both the input data and the model is taken care of by INTISTY.

We now consider the program in more detail, identifying the main steps, the input, and the output. The program and the input are given in Appendix A, and the partial output is given in Appendix B. The first executable statement in MODEL reads in LL, MM, and NN, the components for the positions in the shells, and INDEX, which has a value of 1 through 6 for shells of the type X00, XX0, XXX, XY0, XYY, and XYZ respectively. Note that the shell components have to conform to this arrangement. The variable MUL, specified in the data statement, gives the number of sites for each shell type as identified by INDEX. Variable CT gives the fraction of the sites which are to be 1 atoms and should, for maximum efficiency, correspond to the minor species. In any case, the program labels the 1 atoms as the minor species. TITLE is any identifying text, and ALP are the experimentally determined values of the alphas. A distinction is needed between those alphas which were observed to be zero and those which were not evaluated. The former are to be represented by some small nonzero value, the latter by zero. This distinction is used in evaluating the differences between the observed alphas and those given by the models. The alphas which were not evaluated are not automatically excluded from the design set; exclusion requires a modification to SHELL.

Extensive use is made of the facility of addressing multidimensioned arrays, using a single address. Most often this is done to improve the speed of the computation. In particular, the addresses of all 12,075 sites in IB, which constitute the active volume for modeling, are calculated and listed in LX in loop 1. Loop 2 rearranges these addresses into a random order. RANF is our random number generator which gives numbers uniformly distributed over the interval from zero to one.

The random starting structure is produced by loop 7. The first call to ALPHA provides the counts for the first 28 shells which are needed for the calculation of the components of the design vector. Prior to this count, the random model in IA is transferred into IB. For the first run, SORT is called prior to any modeling and produces the following printout. There are, in effect, 12,075 different fcc cells having six face sites and eight corners. The number of such cells having 0, 1, 2, etc., 1 atoms is determined and printed out. Next a comparison of the populations of various arrangements of 200 neighbors is given. Next is given the joint 110-200 planar population of 1-1 pairs, to be followed by a similar count of planar nonplanar first-neighbor 1-1 pairs. This is followed by the count of the number of 1 atoms having the indicated

joint population of 110, 200, and 211 minor neighbors. In particular, the first position in this table corresponds to the number of 1 atoms having no 1 atoms in any of these three shells.

The last map contains the populations of some of the possible configurations of 1 first neighbors around a 0 atom. The number of 1 atoms is indicated by the numbers which are arranged in the configuration being considered, and all possible orientations are included in the count. When the number replaces the center 0 atom, then this count represents all configurations for that number of 1 atoms not otherwise represented. These configurations have been selected to represent important structures. In particular, the first configuration of four 1 atoms occurs in ordered Cu_3Au , the second results from a shear displacement in the cube face for the same structure, the third occurs in systems which cluster preferentially on cube planes, and the final count gives all other possible configurations. This and the printout for the finished model provide a physical count which may be compared with the populations calculated by Clapp's method.⁴

The modeling is started by executing the statements following statement 11 which select a 0 site. The shell populations and the site location are stored in I00. A 1 site is similarly selected, and the populations are stored in I11 by statements following 13, because initially, V2 has been assigned a large value. If favorable, the interchange of these two atoms will be carried out by a call to 10. Statements following 17 cause a new 0 site to be examined and to replace the first if it is more favorable. If an interchange is not yet possible, a new 1 atom is examined, and the process is carried on until a favorable pair is found. The variables V1, V2, and V3 are the square of the vector length, V1 is for the present model, V2 would result if the two most favorable atoms in the current string were interchanged, and V3 would result if the atom under examination were used. The value of V3 is calculated shell by shell, and any time it is found to exceed V2 the site is abandoned.

An interchange of atoms is carried out by a call to EXCH. In addition, the components of the design vector are adjusted to represent the new configuration. It is necessary that the four layers of atoms immediately surrounding the active volume be adjusted as required, to represent the translations used in replicating the model. Such adjustments are carried out by the subroutine ADJUST. The address of the additional site is given by adding JA, JB, or JC to the location of the site; if no adjustment is required, then JA, JB, or JC are zero.

Two percent of the interchanged pairs will be sufficiently close that they will be related by a shell in the design set. When this occurs, it is necessary to increase the component of the affected shell by unity. It is also necessary to correct V3 (called V in this routine). The

⁴P. C. Clapp, "Atomic Configurations in Binary Alloys," *Phys. Rev. B* 4: 255-70 (1971).

statements between the last call to ADJUST and statement 10 take care of these problems. Should the program be converted to model the bcc lattice, then certain changes would be required in this section.

There are five ways in which the modeling process can be terminated. If a string of 1000 1 sites is examined without an interchange taking place, then the model is terminated. This result is produced by a statement between 13 and 15 in MODEL. This is not a preferred way of termination, since the information concerning the final state is not printed, but it is included to ensure that termination always takes place. Normal termination is caused by V3 being sufficiently small, or the number of interchanges, the modeling time, or the length of scan having reached the specified limits. These tests are indicated on cards B and C, respectively, in EXCH. In the discussion we consider the question of the preferred manner of termination.

For the first model a table is printed which lists the vector components, the elapsed time, and the number of sites which were examined for each block of 100 interchanges. The number of sites is actually one-tenth the true number, and so 20 is the absolute minimum value. This subroutine also accumulates the vector components such that, on completion of modeling, the average rates of change in each shell can be given. Information about the terminal condition is also printed. For the first model this information immediately follows the above table, but for the final models it is listed in a later table. It is possible that the different models can, in some instances, proceed at rather different rates, and the end points may be rather different. The termination information shows whether or not this has occurred. Essentially the same end points being reached will minimize the deviations between models.

During the modeling we have kept track of the changes in the number of 1-1 pairs for the 18 shells, and the number which exists at the finish is calculated and listed in the first line under the comparison of shell populations. This same information is independently given by a call to ALPHA which provides the second line. A failure of these two sets to exactly agree indicates an error in the program, while agreement is almost certain proof that all parts of the program which shift and count atoms are correctly implemented.

After the first model is finished, SORT is again called and gives precisely the same information previously given for the random structure. In some general sense, one can thus see the degree to which the model deviates from the random structure. A printout of 24 of the 25 sheets of atoms in a 21×23 array is produced by a call to DISY. Sites starting as 1 and finishing as 0 are listed as 1 or 2; sites going from 0 to 1, as 3 or 4; and sites remaining 1, as 5 or 6. The even and odd numbers distinguish the two sublattices (with 0's on both), and, as already noted, when these planes are extended by translation, one changes

from one sublattice to the other at the boundaries. The count of the various kinds of atoms is also given. A deck of cards, in the same representation as the printout, is punched in order to save the finished model.

The next table lists the averaged components vs the number of interchanges, while the following table lists the rate of change of these components. These two tables are included to show how the modeling process proceeds. It is found that the components of the higher shells and the shells which have the smaller component reach zero first. Perhaps this is one effect, not two, because the higher shells normally have the smaller components. It also happens that the rate of change can increase and then decrease and that the components will undergo one or more changes in sign. We have generally observed that the first shell is the hardest to complete.

On the next page of the output a table lists the input alphas and the average alphas from the models. The errors in the model alphas are estimated from the deviation from the mean. Provided that all the models are completed by obtaining a short vector length, then the errors in those alphas in the design set must be small, and those for the higher shells will be larger. The average deviation between the observed and model alphas is listed after the table. Note that those alphas which were not determined experimentally and which are represented by zero are excluded from this average.

In some cases it will be physically impossible to obtain models which will reproduce the observed alphas. This can result from the observed alphas being too large in magnitude by a constant factor. A scaling factor which will minimize the difference between the model alphas and the observation is calculated. The average error which would result is also given. Assuming the above difficulty, this can be taken as a rough estimate of the factor to be used to rescale the observations.

A call to INTSTY provides an intensity map for the input alphas as well as for those from the models. Further, using the error estimates and the correlation between the errors for the model, a map of the estimated error for the model intensity is produced. This represents an error estimate based upon the variability in intensity from model to model, and it requires the use of the error correlation for its calculation.

The listed program calculates the intensity for $h_3 = 0$, but it can easily be modified to use other values of h_3 . Modifications may include the use of $h_3 = h_1$ or $h_3 = h_1 + h_2$.

Appendix A contains the listing of the program and the input data. The particular set of alphas have been recently determined for a copper solid solution containing 16 at. % Al.³ Following the data is a second program, COE, which has been written to generate the constants in the

statements in SHELL. The generation of these constants by hand calculations is tedious and prone to error, so this program has been included in case one wants to convert to a bcc lattice or to change the model size.

Appendix B is a partial listing of the output using the listed input. It has been included to illustrate the kind of information generated by the program and for the purpose of identification. However, its most important use is for testing to ensure that the program is properly implemented. Were the program to be implemented precisely in the form listed, the results would be exactly the same. But this requires that the random-number generator produce the same string of numbers as our library function RANF. Using a different string of random numbers, the results of the computations will be similar but not identical.

DISCUSSION

There are three kinds of differences between the present program and the prior program.⁵

The first constitutes refinements and includes the increase in model size, the use of multiple runs to obtain improved accuracy and statistical data, and the inclusion of a larger number of shells in the simulation.

The second kind of changes are those which were made to optimize the computer program. These changes include the use of switching instead of "half switches," thus eliminating the minor composition variations, and the selection of a somewhat different algorithm for deciding on the action to be taken.

The third class constitutes those modifications which represent an extension to the previous program. This includes information about the sequence of events during modeling, the information concerning the configurations produced, and the calculation of the intensity.

The inclusion of many more shells leads to models which better agree with the observations, and this change overshadows possible small differences between the models produced with the present program, compared with our earlier one. Earlier we made several comparisons between our first program and that due to Gehlen and Cohen.⁶ The most important difference identified was that our program could complete a model with significantly

⁵R. O. Williams, *A Computer Program for the Simulation of Solid Solutions from X-Ray Data*, ORNL-TM-2866 (1970).

⁶P. C. Gehlen and J. B. Cohen, "Computer Simulation of the Structure Associated with Local Order in Alloys," *Phys. Rev.* 139: A844-55 (1965).

fewer interchanges. The only point of contact between our present program and the Gehlen-Cohen program as modified by Gragg^{7,8} is contained in Table 1. These alphas were for an aluminum-silver alloy aged 14 hr at 110°C. The second set was produced by their modified program, with the indicated four shells being used in the model. It was stated that while their program continued to interchange the atoms, it appeared that little improvement was resulting. When our program was used with 17 shells, including all members in the table, we obtained the results in the last column. From observations yet to be discussed, we know that we were approaching the limit of the modeling process. Our results are in substantially better agreement with the observations for all shells. Thus, for this case, our program is capable of proceeding considerably further than their program.

⁷

J. E. Gragg, Jr., Ph.D. Thesis, Northwestern University, Evanston, Illinois (1970).

⁸

J. E. Gragg, Jr., and J. B. Cohen, "The Structure of Guinier-Preston Zones in Aluminum-5 at. % Silver," *Acta Met.* 19: 507-19 (1971).

Table 1. Comparison of the Simulation of the
Alphas for an Aged Al-5% As Alloy
Units of alpha $\times$ 1000

Shell	Observed ^a	Gragg-Cohen ^{a,b}	Present Model
110	692	635 ^c	657
200	483	507 ^c	493
211	426		432
200	382	401	379
311	287	348 ^c	291
222	262	287 ^c	266
321	237		231
400	150		165
411	142		150
330	185	195	178
420	130	184	135

^aGragg and Cohen, *Acta. Met.* 19: 507 (1971).

^bGragg, thesis, Northwestern University (1970).

^cUsed in simulation by Gragg.

One normally wants to carry the modeling process essentially to completion but without using excessive time in the terminal stage. This requires setting the limits properly, but for a new set of observations the exact behavior will be unknown. Normally we modify the program so that, for the initial run, only the first model is run with fairly generous limits. Then the best upper limits can be selected and the entire run made. The course of the modeling process is illustrated in Fig. 1 for some typical cases where the vector length and the number of sites per interchange are given vs the number of interchanges. In general, the vector length is not a good limit, since it may not approach zero. And while the rate of improvement per interchange does decrease in the later stages, it would not constitute a sensitive test for the end point. Nor is the time of modeling particularly good, since there will necessarily be some variations between models. The most reliable indication of the approaching end point is the rapid increase in the average scan length per interchange, as may be seen in this figure.

Fig. 1. Three Examples of the Vector Length and the Scan Length vs the Number of Interchanges. The models for the Ni₄Mo and Cu₃Au could not be completed because the input alphas were too large.

Should one care to use either fewer or more interchanges in carrying out the modeling, then one could introduce a biasing term in the comparisons between V1 and V2 and/or V2 and V3. This would have to be done with some care so as not to stop the modeling process.

If one modifies the program such that more than one 0 or 1 site is examined before a comparison is made between V1 and V3, one finds that fewer interchanges are required, because the average improvement per interchange is increased. In the case of Cu-Al, this does not, however, result in a reduction in execution time, nor were significant differences found in the results.

In the present program a single fcc lattice having 12,075 sites and a less regular shape is used in contrast to the two independent fcc lattices having 4000 sites each, a $20 \times 20 \times 20$ cube, as used in the earlier program. This change was made with the thought that the new configuration would have less chance of introducing artifacts due to model size and shape. It is our belief that either size is adequate for representing solid solutions. And they would still be adequate for ordered structures of fine domain size and precipitation systems where the particle size is small. As the number of domains or particles becomes small, perhaps less than ten per model, certain problems of accommodation must surely arise. In this connection it might be noted that modeling which involves particle or domain growth becomes relatively inefficient, because the fraction of the sites which can be favorably interchanged keeps getting smaller and smaller. A solution, when the number of particles or domains can be estimated, is to introduce in the initial model a structure which represents the final structure in terms of the number of particles or domains. The modeling then would consist in taking care of local effects and shape adjustments.

In order to extensively test the present program, we have modeled most of the sets of alphas for fcc solutions which are available. This study is to be published elsewhere, but here we give the results for the Cu-Al alloy (Fig. 2). The correct solution, A, is seen to be reproduced very closely by the model, and in particular we have obtained the splitting in the arms, which was not obtained when the modeling was done with seven shells.⁹ Solution B contains a serious artifact; in particular, this set of alphas gave an intensity of -1.84 at 0.5, 0.5, 0.5. Negative intensities are physically without meaning and cannot occur for a model except from termination effects. The model in this case provided an improved set of alphas (compared with solution B), and the calculated intensity map is fair. Previously when this solution was modeled using six shells, the results were completely unacceptable.

⁹

R. O. Williams, "Short Range Order Structure in a Copper 16 Atomic Percent Aluminum Alloy," *Met. Trans.* 5: 1843-50 (1974).

Fig. 2. Comparison Between the Observed Intensity and the Model Intensity for two Solutions of the Cu-Al Data. The defect in solution B, a large negative value at 0.5, 0.5, 0.5, was corrected by the model; the fit to the intensity in this plane is fair. Previously a seven-shell simulation of solution A failed to give the splitting of the peaks in the arms.

The variability of the alphas is relatively small for the shells in the design set, and in particular, they vanish when the vector length becomes zero. It is further observed that the variability increases for shells which are physically more distant from the design set. This then leads to the situation where the errors in the low alphas are smallest and become progressively larger with higher shells. In fact the error can be rather larger than the values of the alphas for the higher shells. Thus, including all the alphas in the intensity calculation does not introduce questionable structure into the intensity maps, but the maps of the calculated error in the intensity show fine structure associated with the above effect. This problem is, to the best of our knowledge, outside normal statistics considerations, so we do not know its proper treatment. But in any case we are certainly justified in ignoring this fine structure.

We have already mentioned in part the changes which are required to convert the present program into one which models the bcc lattice. A more detailed treatment follows. First, one must change LL, MM, NN, and INDEX to represent the shells for the bcc lattice. The number of shells which can be modeled without major modification is less, specifically only 13. Also MSH, the position of the shells which are in the design set, must be changed. Other changes in the main program are minor, such as dimension changes and the change in format statement 104. In DISY one would make changes so as to identify the four different bcc sublattices.

In SHELL a new set of statements are required, using COE for their generations. ALPHA, ADJUST, and INSTY require no changes beyond possible dimension changes. Common B and D require modifications. All the information generated in SORT applies to the fcc lattice. If similar information is desired for the bcc lattice, then this requires a new program.

If one should desire to increase the size of the model, possibly so as to use more shells in the simulation, then this represents a fairly major effort because of the way in which three-dimensional arrays are addressed with a single address. The modifications can be done only by someone knowledgeable in this technique and also knowledgeable in precisely how the program works. This task should not be undertaken lightly.

The present program, on an IBM 360/91, gives a maximum rate of interchange of 6000/min and an average rate for the Cu-Al data of 4000/min. In particular, the results in the Appendices require 5.5 min, of which 4.8 min was used in the actual modeling.

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Appendix A

Listing of Program and Input Data

For a Copper 16 at. % Al Alloy.


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PROGRAM MODEL
DIMENSION MSH(18), MMM(18), BBI(50,10), BS(50), LX(12075), TITLE(19)
COMMON/8(41,39,29), IA(25,23,21)/G/JA(30), JB(30), JC(30), IC(18,50)
1, JMAX/A/IC(50), LL(50), MM(50), NN(50), MUL(6), INDEX(50)/B/LLL(18), III
2(18), IV, I1(19), I00(19), ITIME, NUM, I100, ISC, ICS, NO, N1, V3/E/ALP(50),
3B(1,50), BSS(50,50)*INTEGER*2IA, IB$DATA(MUL(I), I=1,6)/6,12,8,24,24,
448/, (MSH(I), I=1,18)/1,2,3,4,5,6,7,8,9,10,11,12,13,15,17,19,21,28/
READ103, LL, MM, NN, INDEX*READ100, CT, TITLE
PRINT101, TITLE*READ102, ALP*PRINT105
M=0*DO1I=4,24*IX=I*1599*DO1J=4,26*XL=IX+J*41*DO1K=5,29*MM=M+1*N=L+K
1 LX(M)=N*DO2I=1,12075*IX=12075.*RANF(1.)*1.*IY=LX(IX)*LX(IX)=LX(I)
2 LX(I)=IY*DO4I=1,30*JA(I)=(1-(I+5)/13)*33579*JB(I)=(1-(I+7)/15)*943
4 JC(I)=(1-(I+8)/17)*25*CX=ICC=12075.*CT+.5*CY=12075-ICC*DO5I=1,900
5 IC(I)=0*JMAX=49*DO40I100=1,8*ICS=ISC=NUM=0*DO6I=1,12075
6 IA(I)=0*K=0*DO7I=1,12075*J=12075.*RANF(1.)*1.
IF(IA(J).EQ.1)GOTO7*IA(J)=1*K=K+1*IF(ICC.EQ.K)GOTO8
7 CONTINUE
8 CALL ALPHA(28)*IF(I100.EQ.1)CALLSORT(1)*X=CT/2.*DO9I=1,18*J=MSH(I)
K=MMM(I)=(ALP(J)*CY+CX)*X*FLOAT(MUL(INDEX(J)))+.5*K=LLL(I)=K-IC(J)
9 IC(I,1)=IC(I,1)+K*ITIME=ICLOCK(1.)*IF(I100.EQ.1)PRINT104,LLL
NO=N1=0*V1=V2=1.E20*I1=I2=1*GOTO11
10 ISC=ISC+NO+N1*CALLEXCH*V1=V3*V2=1.E20*IF(NO.LT.0)GOTO31*N1=0
11 I1=I1+1*IF(I1.GT.12075)I1=1*IV=LX(I1)*IF(1B(IV).GT.0)GOTO11
CALLSHELL(1,NX,V2,V3)*NO=1*DO12I=1,19
12 I00(I)=III(I)
13 I2=I2+1*IF(I2.GT.12075)I2=1*IV=LX(I2)*IF(1B(IV).LT.1)GOTO13
N1=N1+1*IF(N1.GT.1000)GOTO31*CALLSHELL(-1,NX,V2,V3)
IF(NX.EQ.0)GOTO16*DO15I=1,19
15 I11(I)=III(I)*V2=V3
16 IF(V3.LT.V1)GOTO10
17 I1=I1+1*IF(I1.GT.12075)I1=1*IV=LX(I1)*IF(1B(IV).GT.0)GOTO17
NO=NO+1*CALLSHELL(0,NX,V2,V3)*IF(NX.EQ.0)GOTO20*DO19I=1,19
19 I00(I)=III(I)*V2=V3
20 IF(V3.LT.V1)GOTO10*GOTO13
31 CALL ALPHA(50)*DO32I=1,50*X=ICC*Y=MUL(INDEX(I))
32 BBI(I,I100)=(FLOAT(IC(I))*24150./CX/Y-CX)/CY
IF(I100.GT.1)GOTO40*DO33I=1,18*III(I)=MMM(I)-LLL(I)
33 LLL(I)=IC(MSH(I))*PRINT109,III,LLL*CALLSORT(0)*CALLOISY
40 CONTINUE*U=V=W=0.*DO42I=1,50*S=0.*DO41J=1,8
41 S=S+BBI(I,J)*Y=BI(I)=S*.125*X=ALP(I)*IF(X.EQ.0.)GOTO42
Z=FLOAT(MUL(INDEX(I)))*T=T+Z*X*X*U=U+Y*Y*Z*V=V+Z*X*Y*W=W+Z
42 CONTINUE*X=V/T*Y=SQRT((T+U-2.*V)/W)*Z=SQRT((U-X*V)/W)
DO45I=1,50*T=PI(I)*DO44J=1,50*U=BI(J)*V=0.*DO43K=1,8
43 V=V+(BBI(I,K)-T)*(BBI(J,K)-U)
44 BSS(I,J)=V
45 BS(I)=SQRT(BSS(I,I)/7.)*PRINT111,(LL(I),MM(I),NN(I),ALP(I),BI(I),
19S(I),I=1,50)*PRINT106,Y,Z,X*CALLINTSTY
100 FORMAT(F4.3,19A4)
101 FORMAT(30X,19A4/)
102 FORMAT(16F5.4)
103 FORMAT(50I1)
104 FORMAT(55H1100 INTERCHANGES/LINE      COMPONENTS OF DESIGN VECTOR ,
160X,16HTIME SCAN VECTOR /9X,105H110      200      211      220      310      222
2      321      400      330      411      420      233      422      431      440      433      244
3      444//6X,18I6)

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105 FORMAT(50H0 CHARACTERIZATION OF RANDCM STARTING STRUCTURE ,//)
106 FORMAT(67H0 AVERAGE WEIGHTED DIFFERENCE BETWEEN OBSERVATIONS AND
1 MODEL IS ,F6.5//22 H THIS IS REDUCED TO ,F8.5,43H IF OBSERVATI
2ONS ARE SCALED BY A FACTOR OF ,F8.5)
109 FORMAT(32H1COMPARISON OF SHELL POPULATIONS,//2(6X,18I6//)34H
1CHARACTERIZATION OF THE MODEL //)
111 FORMAT(60H1 ALPHAS OBSERVED AND FOR THE MODEL, ERRORS FOR THE MO
1DEL //5(10X,3(3I2,3F9.4,5X)//)1)1)SEND

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SUBROUTINE DISYCOMMONIR(41,39,29),IA(25,23,21)*INTEGER*2IB,IA
DIMENSION NUM(25),IZ(8),IX(7)$DATA(IZ(I),I=1,8)/0,1,3,5,0,2,4,6/,
1(IX(I),I=1,7)/7*0/$PRINT101$DO6I=1,25*NUM(I)=I$DO6J=1,23$DO6K=1,21
L=IA(I,J,K)=IZ(IA(I,J,K)+2*IB(I,J,K)+4*MOD(I+J+K,2)+1)$L=L+1
6 IX(L)=IX(L)+1$DO7I J=1,4$I2=I*6$I1=I2-5$IF(IJ.EQ.3)PRINT103
7 PRINT100,(NUM(I),I=I1,I2),(((IA(I,J,K),K=1,21),I=I1,I2),J=1,23)
99 FORMAT(80I1)$PUNCH99,IA
100 FORMAT(1H0,I10,5I22/23(6(1X,21I1//))$PRINT102,IX
101 FORMAT(130H1 MODEL: SITES WHICH WENT FROM 1 TO 0 DURING MODELING
1 ARE PRINTED AS 1 OR 2; FROM 0 TO 1 AS 3 OR 4; AND 1 REMAINING 1 A
2S 5 OR 6. /65H0 THE ODD AND EVEN NUMBERS DISTINGUISH THE TWO FCC
3LATTICES. //)
102 FORMAT(69H0 COUNTS OF NUMBERS OF 0, 1, 2, 3, 4, 5,
1 AND 6 ATOMS. //20X,7I6/1H1)
103 FORMAT(1H1)$RETURN$END

```

```

SUBROUTINESHELL(IX,NX,V2,V3)$INTEGER*2$COMMON(1)/B/M110,M200,M21
11,M220,M310,M222,M321,M400,M330,M411,M420,M233,M422,M431,M440,M433
2,M244,M444,L110,L200,L211,L220,L310,L222,L321,L400,L330,L411,L420
3,L233,L422,L431,L440,L433,L244,L444,J,J1,J2,J3,J4,J5,J6,J7,J8,J9
4,J10,J11,J12,J13,J14,J15,J16,J17,J18,IM,I1,I2,I3,I4,I5,I6,I7,I8,I9
5,I10,I11,I12,I13,I14,I15,I16,I17,I18$NX=0
L110=I(J+1598)+I(J-1598)+I(J+40)+I(J-40)+I(J+1558)+I(J-1558)+I(
1J+1640)+I(J-1640)+I(J+1600)+I(J-1600)+I(J+42)+I(J-42)$IF(IX)1,2,3
1 V3=4.*FLOAT(M110+L110-I1)**2$IF(V3.GT.V2)RETURN$GOTO3
2 V3=4.*FLOAT(M110-L110+J1)**2$IF(V3.GT.V2)RETURN
3 L200=I(J+3198)+I(J-3198)+I(J+82)+I(J-82)+I(J+2)+I(J-2)$IF(IX)4,5,6
4 V3=V3+8.*FLOAT(M200+L200-I2)**2$IF(V3.GT.V2)RETURN$GOTO6
5 V3=V3+8.*FLOAT(M200-L200+J2)**2$IF(V3.GT.V2)RETURN
6 L211=I(J+1556)+I(J-1556)+I(J+1638)+I(J-1638)+I(J+1516)+I(J-1516)+
1I(J+3156)+I(J-3156)+I(J+3238)+I(J-3238)+I(J+1680)+I(J-1680)+
1I(J+1518)+I(J-1518)+I(J+3158)+I(J-3158)+I(J+3240)+I(J-3240)+I(J+16
182)+I(J-1682)+I(J+1560)+I(J-1560)+I(J+1642)+I(J-1642)$IF(IX)7,8,9
7 V3=V3+2.*FLOAT(M211+L211-I3)**2$IF(V3.GT.V2)RETURN$GOTO9
8 V3=V3+2.*FLOAT(M211-L211+J3)**2$IF(V3.GT.V2)RETURN
9 L220=I(J+3196)+I(J-3196)+I(J+80)+I(J-80)+I(J+3116)+I(J-3116)+I(J+3
1280)+I(J-3280)+I(J+3200)+I(J-3200)+I(J+84)+I(J-84)$IF(IX)10,11,12
10 V3=V3+4.*FLOAT(M220+L220-I4)**2$IF(V3.GT.V2)RETURN$GOTO12
11 V3=V3+4.*FLOAT(M220-L220+J4)**2$IF(V3.GT.V2)RETURN
12 L310=I(J+1596)+I(J-1596)+I(J+38)+I(J-38)+I(J+4796)+I(J-4796
1)+I(J+122)+I(J-122)+I(J+1476)+I(J-1476)+I(J+4756)+I(J-4756)+
1I(J+4838)+I(J-4838)+I(J+1722)+I(J-1722)+I(J+4798)+I(J-4798)+I(J+12
14)+I(J-124)+I(J+1602)+I(J-1602)+I(J+44)+I(J-44)$IF(IX)13,14,15
13 V3=V3+2.*FLOAT(M310+L310-I5)**2$IF(V3.GT.V2)RETURN$GOTO15
14 V3=V3+2.*FLOAT(M310-L310+J5)**2$IF(V3.GT.V2)RETURN
15 L222=I(J+3114)+I(J-3114)+I(J+3278)+I(J-3278)+I(J+3118)+I(J-

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13 118)+I(J+3282)+I(J-3282)*IF(IX)16,17,18
16 V3=V3+6.*FLOAT(M222+L222-I6)**2*IF(V3.GT.V2)RETURN$GOTO18
17 V3=V3+6.*FLOAT(M222-L222+J6)**2*IF(V3.GT.V2)RETURN
18 L321=I(J+1514)+I(J-1514)+I(J+3154)+I(J-3154)+I(J+3236)+I(J-3236)+
  I(J+1678)+I(J-1678)+I(J+1474)+I(J-1474)+I(J+4754)+I(J-4754)+
  I(J+4836)+I(J-4836)+I(J+1720)+I(J-1720)+I(J+3074)+I(J-3074)+
  I(J+4714)+I(J-4714)+I(J+4878)+I(J-4878)+I(J+3320)+I(J-3320)+
  I(J+3076)+I(J-3076)+I(J+4716)+I(J-4716)+I(J+4880)+I(J-4880)+
  I(J+3322)+I(J-3322)+I(J+1478)+I(J-1478)+I(J+4758)+I(J-4758)+I(J+
  14840)+I(J-4840)+I(J+1724)+I(J-1724)+I(J+1520)+I(J-1520)+I(J+3160)+
  I(J-3160)+I(J+3242)+I(J-3242)+I(J+1684)+I(J-1684)*IF(IX)19,20,21
19 V3=V3+FLOAT(M321+L321-I7)**2*IF(V3.GT.V2)RETURN$GOTO21
20 V3=V3+FLOAT(M321-L321+J7)**2*IF(V3.GT.V2)RETURN
21 L400=I(J+6396)+I(J-6396)+I(J+164)+I(J-164)+I(J+4)+I(J-4)+
  IF(IX)22,23,24
22 V3=V3+8.*FLOAT(M400+L400-I8)**2*IF(V3.GT.V2)RETURN$GOTO24
23 V3=V3+8.*FLOAT(M400-L400+J8)**2*IF(V3.GT.V2)RETURN
24 L330=I(J+4794)+I(J-4794)+I(J+120)+I(J-120)+I(J+4674)+I(J-4674)+
  I(J+4920)+I(J-4920)+I(J+4800)+I(J-4800)+I(J+126)+I(J-126)+
  IF(IX)25,26,27
25 V3=V3+4.*FLOAT(M330+L330-I9)**2*IF(V3.GT.V2)RETURN$GOTO27
26 V3=V3+4.*FLOAT(M330-L330+J9)**2*IF(V3.GT.V2)RETURN
27 L411=I(J+1554)+I(J-1554)+I(J+1636)+I(J-1636)+I(J+1434)+I(J-1434)+
  I(J+6354)+I(J-6354)+I(J+6436)+I(J-6436)+I(J+1762)+I(J-1762)+I(J+14
  136)+I(J-1436)+I(J+6356)+I(J-6356)+I(J+6438)+I(J-6438)+I(J+1764)+I(
  J-1764)+I(J+1562)+I(J-1562)+I(J+1644)+I(J-1644)*IF(IX)28,29,30
28 V3=V3+2.*FLOAT(M411+L411-I10)**2*IF(V3.GT.V2)RETURN$GOTO30
29 V3=V3+2.*FLOAT(M411-L411+J10)**2*IF(V3.GT.V2)RETURN
30 L420=I(J+3194)+I(J-3194)+I(J+78)+I(J-78)+I(J+6394)+I(J-6394)+
  I(J+162)+I(J-162)+I(J+3034)+I(J-3034)+I(J+6314)+I(J-6314)+
  I(J+6478)+I(J-6478)+I(J+3362)+I(J-3362)+I(J+6398)+I(J-6398)+I(J+16
  16)+I(J-166)+I(J+3202)+I(J-3202)+I(J+86)+I(J-86)*IF(IX)31,32,33
31 V3=V3+2.*FLOAT(M420+L420-I11)**2*IF(V3.GT.V2)RETURN$GOTO33
32 V3=V3+2.*FLOAT(M420-L420+J11)**2*IF(V3.GT.V2)RETURN
33 L233=I(J+3072)+I(J-3072)+I(J+4712)+I(J-4712)+I(J+4876)+I(J-4876)+
  I(J+3318)+I(J-3318)+I(J+4672)+I(J-4672)+I(J+4918)+I(J-4918)+I(J+46
  176)+I(J-4676)+I(J+4922)+I(J-4922)+I(J+3078)+I(J-3078)+I(J+4718)+I(
  J-4718)+I(J+4882)+I(J-4882)+I(J+3324)+I(J-3324)*IF(IX)34,35,36
34 V3=V3+2.*FLOAT(M233+L233-I12)**2*IF(V3.GT.V2)RETURN$GOTO36
35 V3=V3+2.*FLOAT(M233-L233+J12)**2*IF(V3.GT.V2)RETURN
36 L422=I(J+3112)+I(J-3112)+I(J+3276)+I(J-3276)+I(J+3032)+I(J-3032)+
  I(J+6312)+I(J-6312)+I(J+6476)+I(J-6476)+I(J+3360)+I(J-3360)+I(J+30
  136)+I(J-3036)+I(J+6316)+I(J-6316)+I(J+6480)+I(J-6480)+I(J+3364)+I(
  J-3364)+I(J+3120)+I(J-3120)+I(J+3284)+I(J-3284)*IF(IX)37,38,39
37 V3=V3+2.*FLOAT(M422+L422-I13)**2*IF(V3.GT.V2)RETURN$GOTO39
38 V3=V3+2.*FLOAT(M422-L422+J13)**2*IF(V3.GT.V2)RETURN
39 L431=I(J+1472)+I(J-1472)+I(J+4752)+I(J-4752)+I(J+4834)+I(J-4834)+
  I(J+1718)+I(J-1718)+I(J+1432)+I(J-1432)+I(J+6352)+I(J-6352)+
  I(J+6434)+I(J-6434)+I(J+1760)+I(J-1760)+I(J+4632)+I(J-4632)+
  I(J+6272)+I(J-6272)+I(J+6518)+I(J-6518)+I(J+4960)+I(J-4960)+
  I(J+4634)+I(J-4634)+I(J+6274)+I(J-6274)+I(J+6520)+I(J-6520)+
  I(J+4962)+I(J-4962)+I(J+1438)+I(J-1438)+I(J+6358)+I(J-6358)+I(J+64
  140)+I(J-6440)+I(J+1766)+I(J-1766)+I(J+1480)+I(J-1480)+I(J+4760)+I(
  J-4760)+I(J+4842)+I(J-4842)+I(J+1726)+I(J-1726)*IF(IX)40,41,42
40 V3=V3+FLOAT(M431+L431-I14)**2*IF(V3.GT.V2)RETURN$GOTO42

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11 IF(I100.LT.3)PRINT102*PRINT101,I100,NUM,ISC,L,TIME,LLL$JMAX=MINO(N
1,JMAX)$N0=-3*IF(I100.LT.8)RETURN$PRINT103*JM=JMAX+1*DC13II=1,JM
I=I*100-100*DO12JJ=1,18*IX=(IC(JJ,II)+4)/8*IF(IX.LT.1)IX=IX-1
IY=LLL(JJ)*IF(II.GT.1)IC(JJ,II-1)=IX-IY
12 LLL(JJ)=IX
13 PRINT104,I,LLL*PRINT105$DO14I=1,JMAX*J=I*100-50
14 PRINT104,J,(IC(K,I),K=1,18)$RETURN
100 FORMAT(19I6,F6.1,I5,I6)
101 FORMAT(I4,I6,2I8,F7.1,8X,18I5)
102 FORMAT(36H0 CHARACTERISTICS AT END OF MODELING //64H RUN INTCHG
1SCAN VECTOR TIME VECTOR COMPONENTS /)
103 FORMAT(65H0 VECTOR COMPONENTS (AVERAGED) VERSUS THE NUMBER OF INT
1ERCHANGES //27H INTERCHANGES COMPONENTS /)
104 FORMAT(I8,5X,3(I8,4I6),I8,2I6)
105 FORMAT(38H0 RATE OF CHANGE OF VECTOR COMPONENTS //52H INTERCHANGE
1S CHANGE PER 100 INTERCHANGES /)$END

SUBROUTINE ALPHA(NX)$COMMONIB(41,39,29),IA(25,23,21)/A/IC(50),L(50
1),M(50),N(50),MUL(6),INDEX(50)$INTEGER*2IA,IB
IF(NX.GT.30)GOTO6$DO5I=1,41$I I=MOD(I-1,25)+1$DO5J=1,39
JJ=MCD(J-1,23)+1$DO5K=1,29$KK=MOD(K-1,21)+1
5 IB(I,J,K)=IA(II,JJ,KK)$GOTO9
6 DO8K=1,29$DO7J=32,39$JJ=J-23$DO7I=1,33
7 IB(I,J,K)=IB(I,JJ,K)$DO8I=34,41$I I=I-25$DO8J=1,39
8 IB(I,J,K)=IB(II,J,K)
9 DO30II=1,NX$IY=0$GOTO(10,13,16,19,23,24)INDEX(II)
10 J1=L(II)$J2=J1*41$J3=J1*1599$DO12K=1,21$IX=K*1599-1640$DO12J=9,31
IZ=IX+J*41$DO12I=9,33$I0=IZ+I
12 IF( IB(I0).GT.0)IY=IY+IB(I0+J1)+IB(I0+J2)+IB(I0+J3)$GOTO30
13 J1=L(II)$I1=J1*42$I2=J1*40$I3=J1*1600$I4=J1*1598$I5=J1*1558
I6=J1*1640$DO15K=1,21$IX=K*1599-1640$DO15J=9,31$IZ=IX+J*41
DO15I=9,33$I0=IZ+I$IF( IB(I0).GT.0)IY=IY+IB(I0+I1)+IB(I0+I2)+IB(I0+
1I3)+IB(I0+I4)+IB(I0+I5)+IB(I0+I6)
15 CONTINUE$GOTO30
16 J1=L(II)$I1=1557*J1$I2=1559*J1$I3=1639*J1$I4=1641*J1$CO18K=1,21
IX=K*1599-1640$DO18J=9,31$IZ=IX+J*41$DO18I0=9,33$I=IZ+I0
18 IF( IB(I0).GT.0)IY=IY+IB(I0+I1)+IB(I0+I2)+IB(I0+I3)+IB(I0+I4)$GOTO30
19 J1=L(II)$J2=M(II)$J3=J1*41$J4=J2*41$J5=J1*1599$J6=J2*1599
I1=J4+J1$I2=J4-J1$I3=J3+J2$I4=J3-J2$I5=J5+J2$I6=J5-J2
I7=J5+J4$I8=J5-J4$I9=J6+J1$I10=J6-J1$I11=J6+J3$I12=J6-J3
20 DO22K=1,21$IX=K*1599-1640$DO22J=9,31$IZ=IX+J*41$DO22I=9,33$I0=IZ+I
22 IF( IB(I0).GT.0)IY=IY+IB(I0+I1)+IB(I0+I2)+IB(I0+I3)+IB(I0+I4)+IB(I0
1+I5)+IB(I0+I6)+IB(I0+I7)+IB(I0+I8)+IB(I0+I9)+IB(I0+I10)+IB(I0+I11)
2+IB(I0+I12)$GOTO30
23 J1=L(II)$J2=M(II)$J3=J1*41$J4=J2*41$J5=J1*1599$J6=J2*1599
I1=J6+J2+J3$I2=J6-J2+J3$I3=J6-J2-J3$I4=J6+J2-J3
I5=J6+J1+J4$I6=J6-J1+J4$I7=J6-J1-J4$I8=J6+J1-J4
I9=J5+J2+J4$I10=J5-J2+J4$I11=J5-J2-J4$I12=J5+J2-J4$GOTO20
24 J1=L(II)$J2=M(II)$J3=N(II)$J4=J1*41$J5=J2*41$J6=J3*41$J7=J1*1599
J8=J2*1599$J9=J3*1599$I1=J9+J5+J1$I2=J9+J5-J1$I3=J9-J5-J1
I4=J9-J5+J1$I5=J9+J4+J2$I6=J9+J4-J2$I7=J9-J4-J2$I8=J9-J4+J2
I9=J7+J6+J2$I10=J7+J6-J2$I11=J7-J6-J2$I12=J7-J6+J2
I13=J7+J5+J3$I14=J7+J5-J3$I15=J7-J5-J3$I16=J7-J5+J3
I17=J8+J6+J1$I18=J8+J6-J1$I19=J8-J6-J1$I20=J8-J6+J1
I21=J8+J4+J3$I22=J8+J4-J3$I23=J8-J4-J3$I24=J8-J4+J3

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DD26K=1,21*IX=K*1599-1640$DD26J=9,31$IZ=IX+J*41*DD26I=9,33$IO=IZ+I
26 IF(I8(I0).GT.0)
  1IY=IY+I8(I0+I1)+I8(I0+I2)+I8(I0+I3)+I8(I0+I4)+I8(I0+I5)+I8(I0+I6)+
  1I8(I0+I7)+I8(I0+I8)+I8(I0+I9)+I8(I0+I10)+I8(I0+I11)+I8(I0+I12)+
  2I8(I0+I13)+I8(I0+I14)+I8(I0+I15)+I8(I0+I16)+I8(I0+I17)+I8(I0+I18)+
  3I8(I0+I19)+I8(I0+I20)+I8(I0+I21)+I8(I0+I22)+I8(I0+I23)+I8(I0+I24)
30 IC(II)=IY$RETURN$END

SUBROUTINE SORT(IZ) $COMMON I A(41,39,29)/F/LOX,L1X,L21,L2X,L31,L32,
L133,L3X,L41,L42,L43,L4X,L5X,L61,L62,L6X,L7X,L81 $INTEGER*2 I A
DIMENSION N A(7,7),N B(5,5),N C(15),L A(25,7,13),L A1(78),L A2(78),L A3(78
2),N D(6),N E(6),N F(6) $EQUIVALENCE (N D(1),L O X), (N E(1),L 33), (N F(1),L 5X)
N2=N3=N4=L L5=L L6=L L7=0$DO1 I=1,18
1 ND(I)=0$DO2 I=1,2364
2 NA(I)=0$DO3 OI=3,27*II=I-2*I2=I-1*I3=I+1*I4=I+2$DO3 OJ=3,25
  J1=J-2*J2=J-1*J3=J+1*J4=J+2$DO3 OK=3,23$K1=K-2$K2=K-1$K3=K+1$K4=K+2
  N=I A(I1,J1,K1)+I A(I1,J1,K4)+I A(I1,J4,K4)+I A(I1,J4,K1)+I A(I4,J1,K1)
  1+I A(I4,J1,K4)+I A(I4,J4,K4)+I A(I4,J4,K1)+I A(I,J,K2)+I A(I,J,K3)+
  2I A(I,J,K4)+I A(I,J3,K1)+I A(I2,J,K)+I A(I3,J,K)+1$N C(N)=N C(N)+1
  L1=I A(I,J3,K3)*L2=I A(I,J2,K3)$L3=I A(I,J2,K2)*L4=I A(I,J3,K2)
  L5=I A(I3,J3,K)*L6=I A(I2,J3,K)*L7=I A(I2,J2,K)*L8=I A(I3,J2,K)
  L9=I A(I3,J,K3)*L10=I A(I2,J,K3)*L11=I A(I2,J,K2)*L12=I A(I3,J,K2)
  L L=L1+L2+L3+L4+L5+L6+L7+L8+L9+L10+L11+L12+1
  IF(I A(I,J,K).GT.0)GOTO22$GOTO(3,3,5,6,7,8,9,10,11,30,30,30,30)LL
3 ND(LL)=ND(LL)+1$GOTO30
5 IF(L1+L3.EQ.2.OR.L2+L4.EQ.2.OR.L5+L7.EQ.2.OR.L6+L8.EQ.2.OR.L9+L11.
  1EQ.2.OR.L10+L12.EQ.2)GOTO3$LL2X=L2X+1$GOTO30
6 IF(L1+L2+L11+L12.EQ.3.OR.L3+L4+L9+L10.EQ.3.OR.L5+L8+L10+L11.EQ.3.O
  1R.L6+L7+L9+L12.EQ.3.OR.L2+L3+L5+L6.EQ.3.OR.L1+L4+L7+L8.EQ.3)GOTO19
  IF(L3+L6+L9.EQ.3.OR.L1+L8+L11.EQ.3.OR.L2+L11+L5.EQ.3.OR.L7+L4+L9
  1.EQ.3.OR.L3+L5+L10.EQ.3.OR.L1+L7+L12.EQ.3.OR.L4+L8+L10.EQ.3.OR.L2+
  2L6+L12.EQ.3)GOTO20
  IF(L3+L8+L12.EQ.3.OR.L6+L10+L11.EQ.3.OR.L2+L9+L8.EQ.3.OR.L6+L4+L11
  4.EQ.3.OR.L1+L5+L9.EQ.3.OR.L3+L7+L11.EQ.3.OR.L4+L5+L12.OR.L2+L7+L10
  5.EQ.3)GOTO18$LL3X=L3X+1$GOTO30
7 IF(L1+L2+L11+L12.EQ.4.OR.L3+L4+L9+L10.EQ.4.OR.L5+L8+L10+L11.EQ.4.O
  1R.L6+L7+L9+L12.EQ.4.OR.L2+L3+L5+L6.EQ.4.OR.L1+L4+L7+L8.EQ.4)GOTO16
  IF(L1+L2+L3+L4.EQ.4.OR.L5+L6+L7+L8.EQ.4.OR.L9+L10+L11+L12.EQ.4)GOT
  1017$IF(L1+L2+L9+L10.EQ.4.OR.L3+L4+L11+L12.EQ.4.OR.L5+L8+L9+L12.EQ.
  14.OR.L6+L7+L11+L10.EQ.4.OR.L1+L4+L5+L6.EQ.4.OR.L2+L3+L7+L8.EQ.4)GO
  2TO13$LL4X=L4X+1$GOTO30
8 LL5X=LL5X+1$GOTO30
9 LLX=L1+L3+L6+L8+L9+L11$IF(LLX.EQ.6)GOTO15$IF(LLX.EQ.0)GOTO14
  LLX=L2+L4+L5+L7+L9+L11$IF(LLX.EQ.6)GOTO15$IF(LLX.EQ.0)GOTO14$LLX=L1+L3
  1+L5+L7+L10+L12$IF(LLX.EQ.6)GOTO15$IF(LLX.EQ.0)GOTO14$LLX=L2+L4+L6+L8+
  2L10+L12$IF(LLX.EQ.6)GOTO15$IF(LLX.EQ.0)GOTO14$LL6X=L6X+1$GOTO30
10 LL7X=LL7X+1$GOTO30
11 IF(L1+L2+L3+L4.EQ.0.OR.L5+L6+L7+L8.EQ.0.OR.L9+L10+L11+L12.EQ.0)LL81
  1=LL81+1$GOTO30
13 LL43=LL43+1$GOTO30
14 LL62=LL62+1$GOTO30
15 LL61=LL61+1$GOTO30
16 LL42=LL42+1$GOTO30
17 LL41=LL41+1$GOTO30
18 LL33=LL33+1$GOTO30

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19 L32=L32+1$GOTO30
20 L31=L31+1$GOTO30
22 NN=1+IA(I1,J2,K2)+IA(I1,J2,K3)+IA(I1,J3,K3)+IA(I1,J3,K2)
1   +IA(I4,J2,K2)+IA(I4,J2,K3)+IA(I4,J3,K3)+IA(I4,J3,K2)
1   +IA(I2,J1,K2)+IA(I2,J1,K3)+IA(I3,J1,K3)+IA(I3,J1,K2)
1   +IA(I2,J4,K2)+IA(I2,J4,K3)+IA(I3,J4,K3)+IA(I3,J4,K2)
1   +IA(I2,J2,K1)+IA(I2,J3,K1)+IA(I3,J3,K1)+IA(I3,J2,K1)
1   +IA(I2,J2,K4)+IA(I2,J3,K4)+IA(I3,J3,K4)+IA(I3,J2,K4)
M1=IA(I,J,K1)$M2=IA(I,J,K4)$M3=IA(I,J1,K)$M4=IA(I,J4,K)
M5=IA(I1,J,K)$M6=IA(I4,J,K)$MM=M1+M2+M3+M4+M5+M6+1$LA(NN,MM,LL)=
1LA(NN,MM,LL)+1$MA=M1*M2+M3*M4+M5*M6$GOTO(26,26,23,24,25,26,26)MM
23 N2=N2+MA$LL5=LL5+1$GOTO26
24 N3=N3+MA$LL6=LL6+1$GOTO26
25 N4=N4+MA/2$LL7=LL7+1
26 LY=1+M1+M2+M3+M4$LY=1+L1+L2+L3+L4$NB(LX,LY)=NB(LX,LY)+1
LY=1+M3+M4+M5+M6$LY=1+L5+L6+L7+L8$NB(LX,LY)=NB(LX,LY)+1
LY=1+M1+M2+M5+M6$LY=1+L9+L10+L11+L12$NB(LX,LY)=NB(LX,LY)+1
LX=1+L1+L3+L5+L7+L10+L12$LY=LL-LX+1$NA(LX,LY)=NA(LX,LY)+1
LX=1+L1+L3+L6+L8+L9+L11$LY=LL-LX+1$NA(LX,LY)=NA(LX,LY)+1
LX=1+L2+L4+L6+L8+L10+L12$LY=LL-LX+1$NA(LX,LY)=NA(LX,LY)+1
LX=1+L2+L4+L5+L7+L9+L11$LY=LL-LX+1$NA(LX,LY)=NA(LX,LY)+1
30 CONTINUE$PRINT200,NC$PRINT201,LL5,N2,LL6,N3,LL7,N4
PRINT202,NB$PRINT203,NA$DO31I=1,2275
31 IF(LA(I).GT.0)IE=I$IE=(IE/175+1)*175$PRINT204,(LA(I),I=1,IE)
IF(IZ.EQ.1)$READ100,LA1,LA2,LA3$PRINT103,LA1,NC,LA2,NE,LA3,NF
100 FORMAT(78I1)$RETURN
103 FORMAT(86H1 POPULATION OF VARIOUS ARRANGEMENTS OF FIRST NEIGHBOR
1MINOR ATOMS AROUND MAJOR ATOMS/// (I12,5I22/I4,5(I12,I10),I12/I8,5I
222/I6,5(I12,I10),I12/I10,5I22/I2,5(I12,I10),I12/I12,5I22/I4,5(I12,
3I10),I12/I8,5I22/I11,5I22/))
200 FORMAT(104HOCUBE POPULATION- 0 1 2 3 4 5 6
17 8 9 10 11 12 13 14 MINOR ATOMS//16X,15I5/)
201 FORMAT(52H0 CONFIGURATION OF MINOR SPECIES WITH MINOR SPECIES//
19H FOR THE ,I4,28H ATOMS WITH 2 200 NEIGHBORS ,I4,14H ARE IN A LI
2NE,/ 9H FOR THE ,I4,28H ATOMS WITH 3 200 NEIGHBORS , I4,11H AR
3E PLANAR/ 9H FOR THE ,I4,28H ATOMS WITH 4 200 NEIGHBORS , I4,
412H ARE PLANAR.
202 FORMAT(47H0 JOINT POPULATION IN A 110-200 PLANAR COMPLEX//13X,38H
1 0 1 2 3 4 110 NEIGHBORS //5(10X,5I5/))
204 FORMAT(119H1 JOINT 110-200-211 DISTRIBUTION 211'S INCREASE T
10 RIGHT, 110'S INCREASE 1 PER 7 ROWS $ 200'S INCREASE DOWN-RIGHT//
22(7(25I5/1X,25I5/2X,25I5/3X,25I5/4X,25I5/5X,25I5/6X,25I5/))1H1))
203 FORMAT(41H0 JOINT 110 PLANAR-NONPLANAR DISTRIBUTION//24X,44H0 1
1 2 3 4 5 6 PLANAR 110'S//7(20X,7I5/))$END

SUBROUTINE INTSTY
COMMON/A/IC(50),LL(50),MM(50),NN(50),MUL(6),INDEX(50)/E/ALP(50)
1,BI(50),BSS(50,50)$DIMENSIONCO(2200),IX(21,21),IY(21,21),CS(50),IZ
2(21,21)$TWOPI=6.2831853072$H3=0.0$L4=800$L5=400$K=H3*20.+0.01$DH=.0
35$DO60I=1,20$X=I$X=X$COS(TWOPI*X*$DH)$IJ=I-20$DO60J=1,110$IJ=IJ+20
60 CO(IJ)=XX$DO70I1=1,21$I=I1-1$DO70I2=1,21$J=I2-1$TB=TC=0.5
TD=TE=0.$DO68KK=1,50$L=LL(KK)$M=MM(KK)$N=NN(KK)
L1=L*I+L4$L2=L*J+L5$L3=L*K$M1=M*I+L4$M2=M*J+L5$M3=M*K
N1=N*I+L4$N2=N*J+L5$N3=N*K$GOTO(61,62,63,64,65,66)INDEX(KK)
61 TA=CO(L1)+CO(L2)+CO(L3+20)$GOTO67

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62 TA=CO(L1+L2)+CO(L1-L2)+CO(L1+L3)+CO(L1-L3)+CO(L2+L3)
   +CO(L2-L3)*GOTO67
63 TA=CO(L1+L2+L3)+CO(L1+L2-L3)+CO(L1-L2+L3)+CO(L1-L2-L3)*GOTO67
64 TA=CO(L1+M2)+CO(L1-M2)+CO(M1+L2)+CO(M1-L2)+CO(L1+M3)+CO(L1-M3)+CO(
   M1+L3)+CO(M1-L3)+CO(L2+M3)+CO(L2-M3)+CO(M2+L3)+CO(M2-L3)*GOTO67
65 TA=CO(L1+N2+N3)+CO(L1+N2-N3)+CO(L1-N2+N3)+CO(L1-N2-N3)+
   2 CO(L2+N3+N1)+CO(-L2-N3+N1)+CO(L2-N3+N1)+CO(-L2+N3+N1)+
   3 CO(N1+L3+N2)+CO(N1+L3-N2)+CO(N1-L3+N2)+CO(N1-L3-N2)*GOTO67
66 TA= CO(L2+M3+N1)+CO(-L2-M3+N1)+CO(L2-M3+N1)+CO(-L2+M3+N1)+
   2 CO(L1+M2+N3)+CO(L1+M2-N3)+CO(L1-M2+N3)+CO(L1-M2-N3)+
   3 CO(L3+M1+N2)+CO(L3+M1-N2)+CO(-L3+M1+N2)+CO(-L3+M1-N2)+
   4 CO(L3+M2+N1)+CO(-L3+M2+N1)+CO(L3-M2+N1)+CO(-L3-M2+N1)+
   5 CO(L2+M1+N3)+CO(L2+M1-N3)+CO(-L2+M1+N3)+CO(-L2+M1-N3)+
   6 CO(L1+M3+N2)+CO(L1+M3-N2)+CO(L1-M3+N2)+CO(L1-M3-N2)
67 TB=TB+TA*BI(KK)*TD=TD+TA*TA*BSS(KK, KK)*CS(KK)=TA
68 TC=TC+ALP(KK)*TA*TB=TB*200.+5*IF(TB.LT..5)TB=TB-1.*TC=TC*200.+5
   IF(TC.LT..5)TC=TC-1.*IY(I1,I2)=TC*X=0.*DO69LI=1,50$DO69LI=1,50
69 X=X+BSS(LI,LJ)*CS(LI)*CS(LJ)*IZ(I1,I2)=SQRT(X)*75.6+.5
70 IX(I1,I2)=TB$PRINT100,IY$PRINT101,IX$PRINT102,IZ$RETURN
100 FORMAT(1H1/50X,22HEXPERIMENTAL INTENSITY////21(20X,21I4//))
101 FORMAT(1H1/50X,22HINTENSITY FROM MODEL ////21(20X,21I4//))
102 FORMAT(1H1/50X,24HERROR IN MODEL INTENSITY ////21(20X,21I4//))$END

12223234344245454546265656645756627677648867866877
10121220312321324330413242345144352433550144256245
00100210010320110030412012140030351202150141030230
21524361254554662451556465632464556646651556462564
.16 CU-AL DATA FROM PAPER SOLUTION 133 3-19-75 (VERIFIED)
-164 1553 410 302 -605 -335 38 529 -175 232 31 65 -149 -219 68 5
-71 -26 26 217 -74 4 16 70 25 4 -23 4 -8 -25
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0

0000030000000000000003300000200300001020000002000000000000000000303000000
0004403000000044003000400000003000430004440000000400000000000000000000
06000800606000008800600800060600000050067000606000000006008000606000088060008

PROGRAMCDE*DIMENSION L(18),N(18),M(18),IA(48,18),IR(18),NUM(18)
C FOR A IA(I1,I2,I3) MODEL SIZE
READ100,L,M,N*DO1I=1,18$NUM(I)=1$IX=IR(I)=L(I)**2+M(I)**2+N(I)**2
1 PRINT 101,I,L(I),M(I),N(I),IX$IR(10)=50
I1=41$I2=39$I3=29$I2=I1*I2
DO2II=1,9*DO2JJ=1,9$DO2K=1,5$I=II-5$J=JJ-5$IX=I+J*I1+(K-1)*I12
IF(IX.LT.1)GOTO2$IY=I**2+J**2+(K-1)**2
IF(IY.EQ.18.AND.MAXO(IABS(I),IABS(J),IABS(K-1)).EQ.4)IY=50
DO2LL=1,18$IF(IY.NE.IR(LL))GOTO2
IZ=NUM(LL)*NUM(LL)=IZ+2$IA(IZ,LL)=IA(IZ+1,LL)=IX
2 CONTINUE$DO4I=1,18$IX=NUM(I)-1$PUNCH 103,L(I),M(I),N(I)
PRINT 103,L(I),M(I),N(I)$PRINT105,(IA(J,I),J=1,IX)
4 PUNCH105,(IA(J,I),J=1,IX)$PRINT102
100 FORMAT(80I1)
101 FORMAT(I13,3I2,5X,I5)
102 FORMAT(51HOTHER ENDS OF THE PUNCHED STATEMENTS REQUIRE EDITING )
103 FORMAT( 7H L,3I1,1H=)
105 FORMAT(8(5X,1H1,3(4H1(J+,I4,6H)+I(J-,I4,2H)+)/)/)$END
122232343442444424101212203123234344001002100103210344

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Appendix B

Pages 5-9, 11 and 13-15 of the output produced by the program and input data given in Appendix A when the variables on card C, program EXCH have values of 150, 150, and 25 respectively.

100	INTERCHANGES/LINE			COMPONENTS OF DESIGN VECTOR										TIME SCAN VECTOR									
	110	200	211	220	310	222	321	400	330	411	420	233	422	431	440	433	244	444					
	-1596	751	814	316	-1154	-215	98	248	-254	489	12	136	-329	338	29	28	-80	10					
1	-1537	705	736	339	-1076	-193	77	234	-242	470	-15	138	-286	312	40	17	-105	19	1.8	35	4354		
2	-1409	667	681	302	-1039	-176	81	227	-246	443	3	98	-264	298	31	-27	-105	19	3.5	31	4058		
3	-1316	614	646	260	-980	-183	41	202	-203	419	24	69	-220	199	33	-67	-74	36	5.4	35	3767		
4	-1229	562	622	243	-871	-166	1	196	-189	371	-5	103	-194	191	10	-45	-43	55	7.1	33	3485		
5	-1158	515	595	196	-764	-154	29	185	-155	336	-9	131	-174	180	-5	-67	-61	40	9.1	38	3226		
6	-1086	460	591	158	-669	-136	17	157	-143	286	-31	125	-159	164	-6	-76	0	21	11.2	40	2964		
7	-1020	421	523	151	-552	-112	6	144	-145	289	-23	114	-107	86	-27	-53	-17	8	13.4	42	2718		
8	-962	379	478	113	-483	-107	42	110	-98	236	-51	129	-94	86	-24	-21	-34	19	15.4	40	2493		
9	-893	323	413	116	-427	-73	-19	90	-66	182	-25	103	-80	92	-32	-23	-6	9	17.6	41	2239		
10	-802	275	399	72	-382	-77	-20	73	-32	134	-38	102	-59	35	-31	34	19	2	19.9	45	1992		
11	-734	225	316	78	-322	-54	-51	40	-9	141	-49	60	-62	21	-39	23	27	0	22.2	45	1759		
12	-665	176	292	73	-264	-37	-38	18	-1	76	-52	30	-47	42	-33	5	8	7	24.8	53	1546		
13	-597	134	266	56	-217	-26	-65	8	23	67	-24	22	-1	42	-15	0	13	0	27.4	54	1357		
14	-528	78	195	52	-153	-21	4	0	1	31	-24	8	39	31	-11	1	9	19	29.9	53	1145		
15	-441	61	164	47	-96	-13	-35	-6	15	8	-10	26	23	36	-19	14	24	19	32.8	59	949		
16	-362	29	136	44	-81	-14	25	4	-30	13	-6	-6	17	23	-3	7	12	5	36.3	71	772		
17	-303	11	101	36	-62	-13	-4	7	-20	1	-17	4	28	31	12	-13	18	3	38.9	57	640		
18	-236	-10	56	30	-25	-9	1	-3	2	-28	-14	21	11	-5	-12	-11	5	-14	42.3	72	490		
19	-175	-3	33	30	-26	2	16	-5	-5	-19	-8	-3	-14	13	-8	-4	2	-6	46.3	86	364		
20	-125	-9	22	13	-7	3	20	2	-6	-6	1	-2	8	-3	-3	5	5	2	50.5	98	257		
21	-72	-10	2	3	5	7	8	-1	7	4	-17	-14	6	5	-9	4	-11	2	54.9	100	155		
22	-26	-3	10	0	-5	0	-6	-1	4	-8	-4	2	-4	11	1	2	3	2	61.5	152	59		

CHARACTERISTICS AT END OF MODELING

RUN	INTCHG	SCAN	VECTOR	TIME	VECTOR COMPONENTS																	
1	2200	12786	59	61.5	-26	-3	10	0	-5	0	-6	-1	4	-8	-4	2	-4	11	1	2	3	2

COMPARISON OF SHELL POPULATIONS

280	1686	4498	2149	2536	1019	7573	1186	1680	4169	3774	3834	3423	7673	1785	3758	3562	1237
280	1686	4498	2149	2536	1019	7573	1186	1680	4169	3774	3834	3423	7673	1785	3758	3562	1237

CHARACTERIZATION OF THE MODEL

CUBE POPULATION-	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	MINOR ATOMS
	798	2826	3799	2719	1360	436	114	21	2	0	0	0	0	0	0	

CONFIGURATION OF MINOR SPECIES WITH MINOR SPECIES

FOR THE 665 ATOMS WITH 2 200 NEIGHBORS 138 ARE IN A LINE
 FOR THE 336 ATOMS WITH 3 200 NEIGHBORS 199 ARE PLANAR
 FOR THE 98 ATOMS WITH 4 200 NEIGHBORS 22 ARE PLANAR.

JOINT POPULATION IN A 110-200 PLANAR COMPLEX

	0	1	2	3	4	110 NEIGHBORS
1182	262	14	0	0		
2168	217	2	0	0		
1484	49	0	0	0		
381	0	0	0	0		
37	0	0	0	0		

JOINT 110 PLANAR-NONPLANAR DISTRIBUTION

	0	1	2	3	4	5	6	PLANAR 110'S
5612	996	21	0	0	0	0	0	
996	82	0	0	0	0	0	0	
21	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	
0	0	0	0	0	0	0	0	

211'S INCREASE TO RIGHT, 110'S INCREASE 1 PER 7 ROWS & 200'S INCREASE DCWN-RIGHT

31

POPULATION OF VARIOUS ARRANGEMENTS OF FIRST NEIGHBOR MINOR ATOMS AROUND MAJOR ATOMS

MODEL: SITES WHICH WENT FROM 1 TO 0 DURING MODELING ARE PRINTED AS 1 OR 2; FROM 0 TO 1 AS 3 OR 4; AND 1 REMAINING 1 AS 5 OR 6.
THE ODD AND EVEN NUMBERS DISTINGUISH THE TWO FCC LATTICES.

1	2	3	4	5	6
000000402020000020050	000000000210020000500	000001000000010160032	003030020000005210000	404140000303000063000	001000060004005400000
060000001030300200000	000000006061000500000	560010003250500050000	010000404040406000000	500002300000000200020	00000000000002100430
000061410000000000000	000050301200043000005	010000000000000040404	003036000000000000323	002000000065252501000	000430065050041000000
061002000010000406020	250000010500000003000	060410040610300200003	010000303010040000002	361000020000000010000	400000000100200000030
400061602060000000000	000000001000020400100	000503000003610000012	100204020010003030540	000105204305430060400	000014100000000000020
001030305000000206020	004020000300004303050	300002040000000000001	000000000040006021010	305632001000000000105	000000000040010003000
402000000003452001000	001200000000010020000	400543000005650040000	100210101000000052000	432021206500030040400	100000000000000000000
063200303200000400061	030001604040002503006	001000123000000000020	006300610000006000450	100002000001000300000	000565250000000000000
000540002000230000012	000000000230040000003	400000010000000120010	021000000000023000000	012020006000000040006	00000002000000002525
000000000006004000000	25600300000000300004	000000000300004060000	054105050000400003050	040210000012000006000	000505000000056505000
000000000001000000010	1006040630000501000303	000300012001000020002	000200040002000050000	000100000300032001000	000000004040000100000
020000300632040402020	030000202120010001406	040000020400005010000	030000002103004000000	060434100000000000303	000000002000002300000
000041000000030303002	000002000000000000020	010040032023000040000	000002040006000000001	200000000001000000000	000000040404000004040
100000000400001202100	436503000320060006060	020000000200010505000	010041000001004001604	040030003452305030320	030000000000000000050
600060030005232143000	000000041000000000000	000100050003600040000	005000020000000200003	00000000020000000002	100000040600000016060
300002000004040000040	004303000000010100600	000400020000345000300	000003412000000000402	500002100034003000321	006525200000000001000
0021010000000000001002	000200103432000400000	030000000602000200060	003000000000000000005	004000030000004140000	000000040000100000003
503212000002143056040	400020600000000000000	000000300030500004000	400041404020600503404	000000000050300000300	000000000101000000000
000100050003200001000	001010000004000402000	000000000020000000200	005032023000000202000	002000000000000040000	061404041400000000040
000000101400020004000	000503400000050500006	000002100400060010300	000160410020050000000	300000000214041000503	000123000103206300010
000040200040200003200	040000000230000000003	000000000001000000000	000200501000003000043	000000000300000003000	103004060602000010040
000010000000025000520	000000000000000001402	300000100406340034000	006000610000000001000	300400000204560002000	000000030100010560000
400040000100610040000	023450045030100200030	000000010000000000050	000050523030003000021	6020000000000010000030	020050000030000000000

7	8	9	10	11	12
200003000300210005030	000400000006000000000	000160650000002140012	000000000214000010000	000000000000000020010	040200000400101000023
363004100000300000000	000000000100616300400	003000000000000000020	406023000500000303050	300000043000020012000	206000010000606040002
032001000020000001002	100600123030000000320	000040406000000002010	100000100000040406001	000340200040002000000	000200003050000030303
001000340600303030100	000000000000004000000	543050300010003000040	000000200503002105050	5400100200000023000040	010020000001004000000
030500000000010000006	000006003030300000500	000000000000000061600	020406000000000002000	000000004000000060002	005050005030300200303
040630301000020604020	000100000001000300000	503030340002100200000	000000200540030000002	300002500000000050060	00000000000400000200
050001204003003010006	000206000050040000000	000001000100000100000	0000040002001402000505	030300000000202000010	000004040012000000300
000000100006000604000	004505030000030000002	100200000006000404145	006505000000000000000	00020000204020200040	010005000020000500000
230000606000000000060	500400100000060000500	000000606000010000210	040000000050540450520	000000036000000000000	500000001430561006540
000000030000002000000	000301000000050300000	000010323000100004000	200040002020000000000	100010020006000000003	000040000000004000000
234000000030001406000	000000000002000000503	000001200305012000000	563200000404540030005	000000036500000060402	04000000000000002300
000036500200001000000	000000004000450000000	140434020000034040000	000100010000010021000	000030100000003000000	000060400005000500000
004000003050160050000	503000000010000250040	010100000000000000000	000010001602500050000	406020050000604043054	000000000000000010100
000050301000023200000	000000606040410100000	000000000050100000005	000340000021004001400	000000000000230000000	000345600000000000200
600001002303200020000	00000000000120000060	054003030000003030000	300000004000000000001	404000006005402020002	100000005004001000001
001000001000005050300	200303206000040600000	000000000006020010020	000000200000010040030	001000000000300202000	000365410000000045000
03000000540000000606	041400000000020000005	00000230505050301600	000004020400001000000	450000000000004500404	060000000030100002000
023050300000003052000	000001006040040400000	030303000000000202300	000000004003000001000	000030000004000010000	000000400000000005000
230120200000402000030	100200120050305010041	416020010020020002000	000000503000000450020	036040210000000000434	005000300010060600000
000200100000000004000	000545634005006000000	500000000000040004500	000300404005010000200	000010000000000000500	000000000000000001000
404000010320030005000	001000000002000002000	004100000000000001000	000000030100034001000	056060000100400000000	022034043400000606060
000002000010501000000	030305030000004000000	000600040002501000500	050500002000206000000	001000301030000010300	000001000000010100000
012000000340010003034	000004000010003000000	000000000040400040606	040000103010005010020	002040416040400061404	060030005200105050103

CHARACTERISTICS AT END OF MODELING

RUN	INTCHG	SCAN	VECTOR TIME		VECTOR COMPONENTS																	
2	2311	13169	38	65.6	-10	-2	1	0	-1	1	3	1	1	-3	4	6	2	-4	1	1	2	0
3	2332	13173	62	64.5	-9	-2	1	0	3	2	-2	-1	-2	-4	7	-1	1	-3	-1	1	-3	-2
4	2319	13337	46	68.2	-10	1	-3	3	-2	0	4	-1	0	-2	2	-2	1	0	-1	2	6	0
5	2353	13000	81	66.4	-9	-2	-1	-1	-1	2	2	-2	0	-6	-4	0	-2	-8	1	2	1	0
6	2246	12298	66	63.4	-9	-1	3	-1	-1	0	-2	0	-2	-3	-6	6	-1	1	-1	2	-2	1
7	2253	12418	81	62.6	-8	0	-2	2	-5	2	-2	1	1	-2	-3	-2	3	0	-2	6	-3	1
8	2200	13304	33	65.3	-14	1	3	1	-2	3	3	-2	-1	4	-5	0	0	-2	2	-3	1	-2

VECTOR COMPONENTS (AVERAGED) VERSUS THE NUMBER OF INTERCHANGES

INTERCHANGES	COMPONENTS																			
0	-1605	760	810	305	-1188	-225	123	250	-166	440	68	90	-295	239	-62	36	-116	-8		
100	-1519	718	763	299	-1121	-213	119	235	-156	428	66	86	-277	240	-56	22	-115	-1		
200	-1424	676	720	277	-1054	-196	120	219	-153	389	66	67	-251	228	-59	18	-115	2		
300	-1337	631	672	249	-988	-187	113	201	-138	362	66	70	-230	210	-64	16	-116	3		
400	-1263	580	627	231	-906	-177	80	189	-130	335	45	69	-217	189	-61	35	-114	12		
500	-1185	532	580	197	-827	-160	71	174	-113	302	30	72	-199	183	-52	18	-104	7		
600	-1113	478	542	172	-759	-147	55	152	-102	271	19	72	-174	151	-38	4	-67	3		
700	-1040	433	500	166	-665	-126	34	139	-93	241	13	67	-128	113	-34	-4	-37	3		
800	-975	376	457	143	-582	-110	6	114	-78	212	-8	70	-96	95	-40	-12	-36	6		
900	-904	332	417	134	-499	-97	-6	96	-50	163	-4	44	-53	47	-24	-7	-22	10		
1000	-835	276	371	109	-416	-82	-5	76	-35	105	2	22	-36	16	-25	-9	-10	9		
1100	-762	219	344	80	-339	-78	5	53	-26	87	-23	17	-21	-1	-40	9	6	9		
1200	-692	167	315	64	-276	-57	2	44	-6	58	-34	4	-7	7	-39	-4	15	-1		
1300	-619	126	284	49	-228	-41	-15	30	5	41	-26	-20	6	25	-34	-16	27	-7		
1400	-548	94	226	48	-182	-20	-22	21	6	29	-18	-32	-1	38	-36	-7	13	-2		
1500	-470	68	201	38	-130	-11	-28	16	2	-7	-9	-15	-1	34	-32	8	18	1		
1600	-399	50	146	41	-103	-4	-26	10	-10	-10	-19	-14	4	17	-17	5	12	-1		
1700	-327	29	127	43	-77	-5	-8	3	-11	-6	-17	-1	10	-10	-8	3	25	1		
1800	-266	6	92	33	-38	-2	-1	-4	-1	-13	-21	-4	9	-14	-17	-1	7	-1		
1900	-208	-5	61	29	-20	3	-1	-4	-9	-17	-25	-8	-2	-4	-11	6	10	2		
2000	-152	-1	38	19	-13	3	5	1	-7	-6	-14	-1	9	-4	-10	-2	9	1		
2100	-99	-2	17	9	-10	-1	7	1	2	-2	-1	-1	7	-6	-2	-1	3	4		
2200	-49	-3	13	3	-4	2	4	-2	-1	-3	-5	-2	1	-5	1	2	3	-1		

RATE OF CHANGE OF VECTOR COMPONENTS

INTERCHANGES	CHANGE PER 100 INTERCHANGES																			
50	86	-42	-47	-6	67	12	-4	-15	10	-12	-2	-4	18	1	6	-14	1	7		
150	95	-42	-43	-22	67	17	1	-16	3	-39	0	-19	26	-12	-3	-4	0	3		
250	87	-45	-48	-28	66	9	-7	-18	15	-27	0	3	21	-18	-5	-2	-1	1		
350	74	-51	-45	-18	82	10	-33	-12	8	-27	-21	-1	13	-21	3	19	2	9		
450	78	-48	-47	-34	79	17	-9	-15	17	-33	-15	3	18	-6	9	-17	10	-5		
550	72	-54	-38	-25	68	13	-16	-22	11	-31	-11	0	25	-32	14	-14	37	-4		
650	73	-45	-42	-6	94	21	-21	-13	9	-30	-6	-5	46	-38	4	-8	30	0		
750	65	-57	-43	-23	83	16	-28	-25	15	-29	-21	3	32	-18	-6	-8	1	3		
850	71	-44	-40	-9	83	13	-12	-18	28	-49	4	-26	43	-48	16	5	14	4		
950	69	-56	-46	-25	83	15	1	-20	15	-58	6	-22	17	-31	-1	-2	12	-1		
1050	73	-57	-27	-29	77	4	10	-23	9	-18	-25	-5	15	-17	-15	18	16	0		
1150	70	-52	-29	-16	63	21	-3	-9	20	-29	-11	-13	14	8	1	-13	9	-10		
1250	73	-41	-31	-15	48	16	-17	-14	11	-17	8	-24	13	18	5	-12	12	-6		
1350	71	-32	-58	-1	46	21	-7	-9	1	-12	8	-12	-7	13	-2	9	-14	5		
1450	78	-26	-25	-10	52	9	-6	-5	-4	-36	9	17	0	-4	4	15	5	3		
1550	71	-18	-55	3	27	7	2	-6	-12	-3	-10	1	5	-17	15	-3	-6	-2		
1650	72	-21	-19	2	26	-1	18	-7	-1	4	2	13	6	-27	9	-2	13	2		

ALPHAS OBSERVED AND FOR THE MODEL, ERRORS FOR THE MODEL

1 1 0	-0.1644	-0.1632	0.0006	2 0 0	0.1553	0.1554	0.0003	2 1 1	0.0410	0.0409	0.0002
2 2 0	0.0302	0.0302	0.0001	3 1 0	-0.0605	-0.0604	0.0001	2 2 2	-0.0335	-0.0337	0.0002
3 2 1	0.0038	0.0038	0.0001	4 0 0	0.0529	0.0530	0.0002	3 3 0	-0.0175	-0.0175	0.0002
4 1 1	0.0232	0.0233	0.0002	4 2 0	0.0031	0.0032	0.0002	2 3 3	0.0065	0.0064	0.0002
4 2 2	-0.0149	-0.0149	0.0001	5 1 0	-0.0219	-0.0210	0.0018	4 3 1	0.0068	0.0068	0.0001
5 2 1	0.0005	-0.0010	0.0015	4 4 0	-0.0071	-0.0071	0.0001	5 3 0	-0.0026	-0.0039	0.0015
4 3 3	0.0026	0.0025	0.0001	6 0 0	0.0217	0.0166	0.0092	2 4 4	-0.0074	-0.0074	0.0002
6 1 1	0.0004	0.0075	0.0044	5 3 2	0.0016	0.0019	0.0017	6 2 0	0.0070	0.0041	0.0034
5 4 1	0.0025	0.0018	0.0016	6 2 2	0.0004	-0.0030	0.0047	6 3 1	-0.0023	0.0013	0.0035
4 4 4	0.0004	0.0004	0.0002	5 5 0	-0.0008	0.0026	0.0063	7 1 0	-0.0025	-0.0064	0.0028
5 4 3	0.0	-0.0000	0.0013	6 4 0	0.0	-0.0012	0.0043	6 3 3	0.0	-0.0002	0.0038
2 5 5	0.0	0.0017	0.0023	7 2 1	0.0	-0.0011	0.0019	6 4 2	0.0	-0.0015	0.0030
7 3 0	0.0	-0.0012	0.0028	7 3 2	0.0	0.0014	0.0024	6 5 1	0.0	-0.0010	0.0039
4 5 5	0.0	-0.0005	0.0009	8 0 0	0.0	0.0077	0.0076	8 1 1	0.0	-0.0001	0.0027
6 4 4	0.0	-0.0005	0.0028	7 4 1	0.0	-0.0008	0.0015	8 2 0	0.0	0.0029	0.0046
6 5 3	0.0	-0.0005	0.0024	6 6 0	0.0	0.0003	0.0061	8 2 2	0.0	-0.0002	0.0038
7 4 3	0.0	-0.0002	0.0012	7 5 0	0.0	0.0017	0.0048				

AVERAGE WEIGHTED DIFFERENCE BETWEEN OBSERVATIONS AND MODEL IS .00211

THIS IS REDUCED TO 0.00210 IF OBSERVATIONS ARE SCALED BY A FACTOR OF 0.99394

EXPERIMENTAL INTENSITY

20	21	23	24	22	24	38	54	101	207	274	207	101	54	38	24	22	24	23	21	20
21	22	24	25	24	27	40	56	109	227	300	227	109	56	40	27	24	25	24	22	21
23	24	27	29	29	33	46	67	138	284	371	284	138	67	46	33	29	29	27	24	23
24	25	29	33	34	40	55	82	166	325	417	325	166	82	55	40	34	33	29	25	24
22	24	29	34	38	47	65	91	164	297	373	297	164	91	65	47	38	34	29	24	22
24	27	33	40	47	60	80	107	168	270	327	270	168	107	80	60	47	40	33	27	24
38	40	46	55	65	80	105	142	212	317	373	317	212	142	105	80	65	55	46	40	38
54	56	67	82	91	107	142	187	258	361	417	361	258	187	142	107	91	82	67	56	54
101	109	138	166	164	168	212	258	289	339	371	339	289	258	212	168	164	166	138	109	101
207	227	284	325	297	270	317	361	339	306	300	306	339	361	317	270	297	325	284	227	207
274	300	371	417	373	327	373	417	371	300	274	300	371	417	373	327	373	417	371	300	274
207	227	284	325	297	270	317	361	339	306	300	306	339	361	317	270	297	325	284	227	207
101	109	138	166	164	168	212	258	289	339	371	339	289	258	212	168	164	166	138	109	101
54	56	67	82	91	107	142	187	258	361	417	361	258	187	142	107	91	82	67	56	54
38	40	46	55	65	80	105	142	212	317	373	317	212	142	105	80	65	55	46	40	38
24	27	33	40	47	60	80	107	168	270	327	270	168	107	80	60	47	40	33	27	24
22	24	29	34	38	47	65	91	164	297	373	297	164	91	65	47	38	34	29	24	22
24	25	29	33	34	40	55	82	166	325	417	325	166	82	55	40	34	33	29	25	24
23	24	27	29	29	33	46	67	138	284	371	284	138	67	46	33	29	29	27	24	23
21	22	24	25	24	27	40	56	109	227	300	227	109	56	40	27	24	25	24	22	21
20	21	23	24	22	24	38	54	101	207	274	207	101	54	38	24	22	24	23	21	20

INTENS ITY FROM MODEL

15	21	32	28	25	29	37	66	99	182	252	182	99	66	37	29	25	28	32	21	15
21	22	28	26	26	29	36	63	102	211	297	211	102	63	36	29	26	26	28	22	21
32	28	27	29	31	33	44	76	135	281	387	281	135	76	44	33	31	29	27	28	32
28	26	29	35	38	39	53	90	161	309	409	309	161	90	53	39	38	35	29	26	28
25	26	31	38	46	51	59	94	164	291	372	291	164	94	59	51	46	38	31	26	25
29	29	33	39	51	61	73	111	179	289	358	289	179	111	73	61	51	39	33	29	29
37	36	44	53	59	73	95	135	201	307	372	307	201	135	95	73	59	53	44	36	37
66	63	76	90	94	111	135	178	255	354	409	354	255	178	135	111	94	90	76	63	66
99	102	135	161	164	179	201	255	323	368	387	368	323	255	201	179	164	161	135	102	99
182	211	281	309	291	289	307	354	368	324	297	324	368	354	307	289	291	309	281	211	182
252	297	387	409	372	358	372	409	387	297	252	297	387	409	372	358	372	409	387	297	252
182	211	281	309	291	289	307	354	368	324	297	324	368	354	307	289	291	309	281	211	182
99	102	135	161	164	179	201	255	323	368	387	368	323	255	201	179	164	161	135	102	99
66	63	76	90	94	111	135	178	255	354	409	354	255	178	135	111	94	90	76	63	66
37	36	44	53	59	73	95	135	201	307	372	307	201	135	95	73	59	53	44	36	37
29	29	33	39	51	61	73	111	179	289	358	289	179	111	73	61	51	39	33	29	29
25	26	31	38	46	51	59	94	164	291	372	291	164	94	59	51	46	38	31	26	25
28	26	29	35	38	39	53	90	161	309	409	309	161	90	53	39	38	35	29	26	28
32	28	27	29	31	33	44	76	135	281	387	281	135	76	44	33	31	29	27	28	32
21	22	28	26	26	29	36	63	102	211	297	211	102	63	36	29	26	26	28	22	21
15	21	32	28	25	29	37	66	99	182	252	182	99	66	37	29	25	28	32	21	15

1- 2.	Central Research Library	25.	H. Postma
3.	Document Reference Section	26.	C. J. Sparks
4-13.	Laboratory Records Department	27.	D. B. Trauger
14.	Laboratory Records, ORNL RC	28.	J. R. Weir, Jr.
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