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Computer Programs for Structural Chemistry:

MATCH1 and MATCH2, FORTRAN Programs To Predict and Evaluate Mutual Orientation of Polycrystals

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Table of Contents

Computer Programs for Structural Chemistry: MATCH1 and MATCH2, FORTRAN programs to predict and evaluate mutual orientation of polycrystals [+]

Brian Dickens and LeRoy W. Schroeder*

Two computer programs to evaluate possible structural matches for use in epitaxy and twinning studies have been written in FORTRAN V for the UNIVAC 1108. They should be readily convertible to other comparable computers.

The first program, MATCH1, requires knowledge of the unit cell parameters. It obtains all matching networks in two unit cell lattices and sorts the matches into an order of probable epitaxy (or twinning if the two unit cells are the same) based solely on criteria of dimensional mismatch and network area.

The second program, MATCH2, requires knowledge of positional parameters of the atoms in the crystal structures. It calculates the degree of structural fit for slices supplied from visual inspection of the crystal structures or as matching networks determined by MATCH1.

The slice comparison is carried out in terms of the vector set of the environment of each atom in each slice. The procedure is not valid when the twin operation is a rotation about the normal of the compositional plane or a reflection in a mirror parallel to this plane. The atomic patterns comprising the slices are matched piece by piece in MATCH2. A third program, MATCH3, will match whole patterns once three fiducial atoms in each pattern have been picked from the output of MATCH2 and will handle all the twinning cases.

This Technical Note explains the procedure in MATCH1 and MATCH2 and includes examples of results. The programs are available on magnetic tape or card decks obtainable from the authors.

Key words: Computer calculations; crystal structure; epitaxy; lattice misfit; pattern recognition; twinning

[+] To obtain a microfiche copy of this Technical Note and the FORTRAN code listings, please contact the Input Section, National Technical Information Service, Springfield, Va. 22151.

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Introduction

The phenomenon of regular mutual orientation of component crystals of various substances in polycrystals is widely spread and is encountered by workers in the fields of solid state chemistry, metallurgy and materials research. Regular mutual orientation of crystals of two (or more) phases sharing a common surface arises during crystallization and is assumed to be controlled by structural analogies between the crystalline phases.

Polycrystals give rise to several effects important in solid state chemistry and precipitation processes:

1. apparent nonstoichiometry,
2. apparent impurity incorporation,
3. seeding of anhydrous salts or low hydrates in aqueous environments via epitactical growth on highly hydrated precursors, and
4. topotaxy, in which the products of solid state reactions have a regular crystallographic orientation with respect to the reactant crystal.

We have been concerned with assessing _a priori_ the possibilities of polycrystal formation via intergrowths or overgrowths of calcium phosphates. _A priori_ assessment has proved necessary because of experimental difficulties. Calcium phosphates do not lend themselves to vapor deposition techniques because some calcium phosphates decompose under even mildly adverse conditions. Also, some intermediate phases such as high hydrates acting as seed templates have only a transient existence under biological conditions. There are, however, several examples in the field of calcium phosphates where two intergrown phases have both survived to produce a polycrystal of macroscopic size. We believe it is possible and meaningful in many cases to investigate the structural relationship of the various stable phases in polycrystals regardless of any intermediate phases. Hence, we have devised the procedures described in this publication.

Growth of calcium phosphates from solution in situations such as precipitation of a more stable phase with dissolution of a less stable phase usually takes place under conditions of only slight supersaturation. The degree of structural misfit which can be accommodated under these gentle conditions is probably smaller than misfits possible under more drastic conditions such as vapor deposition of a thin film onto a substrate. Thus, "chemical" fits of the parts of the calcium phosphate structures actually in contact with one another are probably very important, because of (i) the smaller thermodynamic driving force in deposition from solution vis-a-vis vapor, and (ii) the necessity of interlocking patterns of monatomic and polyatomic ions which differ considerably in size and local charge.

To study the importance and extent of occurrence of polycrystal formation in calcium phosphate chemistry in a systematic and objective way while considering all reasonable possibilities, we have written (in FORTRAN V) the computer programs MATCH1 and MATCH2 described here.

The major innovations in our approach are:

(1) All reasonable and unique metric fits between two-dimensional networks in two three-dimensional lattices are calculated. The reasonableness of the misfit is based on quantitative criteria of allowed misfit and on the maximum allowed dimension in the networks. Subsequently, these network matches are sorted into an order of probable matching based on misfit of the component lengths and angles and on the area of each network plane.

(2) For each of the most probable network-network matches obtained in step (1), we calculate quantitative figures of merit based on the degree of structural fit of corresponding atom locations and charges in thin slices which may be capable of replacing one another. The atomic details are obtained from known crystal structures.

(3) Our approach is one of filtering, in that surviving cases are possible but not definite cases. In general this approach is necessary to save computer time. A pre-conceived case can be tested at the higher level structural-fit gauging stage. To be even more diagnostic, we are writing a third stage which places the two components of the contact layer in juxtaposition. This stage removes the limitations (discussion on p. 17) of the 'incomplete filtering' in our present approach.

Overview of MATCH1 and MATCH2

The rationale in step (1) of the introduction forms the basis of our program MATCH1. Networks are generated by pairing vectors of the type $\underset{\sim}{r} = u\underset{\sim}{a} + v\underset{\sim}{b} + w\underset{\sim}{c}$ where $\underset{\sim}{a}$, $\underset{\sim}{b}$ and $\underset{\sim}{c}$ are the primitive vectors. Values of u, v and w of -4 to +4 are generated to create each lattice vector, r. The crystal form is consistent with the symmetry of the point group. Also any set of planes through the crystal structure must be consistent with this symmetry. Point group symmetry is applied to remove redundant values of u, v and w. Thus, a network for compound A would be based on vectors $\underset{\sim}{r}_{A1}$ and $\underset{\sim}{r}_{A2}$ and on $\underset{\sim}{r}_{B1}$ and $\underset{\sim}{r}_{B2}$ for compound B. Vectors are paired if the lengths agree within 15%. Thus the two networks would be represented as $(\underset{\sim}{r}_{A1}, \underset{\sim}{r}_{A2})$ and $(\underset{\sim}{r}_{B1}, \underset{\sim}{r}_{B2})$ where $\underset{\sim}{r}_{A1}$ is paired with $\underset{\sim}{r}_{B1}$ and $\underset{\sim}{r}_{A2}$ with $\underset{\sim}{r}_{B2}$. The unit meshes represented by these networks are rotated to closest coincidence. A generalized misfit is then calculated as $2|\Delta\underset{\sim}{r}_{+}|/|\underset{\sim}{r}_{A1}+\underset{\sim}{r}_{A2}|$ and $2|\Delta\underset{\sim}{r}_{-}|/|\underset{\sim}{r}_{A1}-\underset{\sim}{r}_{A2}|$ where $\Delta\underset{\sim}{r}_{+}$ and $\Delta\underset{\sim}{r}_{-}$ are vectors from the mesh point in network A to the corresponding mesh point in network B, e.g., $\Delta\underset{\sim}{r}_{+} = \underset{\sim}{r}_{A1} + \underset{\sim}{r}_{A2} - (\underset{\sim}{r}_{B1}+\underset{\sim}{r}_{B2})$. An estimate of the corresponding misfit dislocation on density is given by

$$(\big||\underset{\sim}{r}_{A1}|-|\underset{\sim}{r}_{B1}|\big|)(\big||\underset{\sim}{r}_{A2}|-|\underset{\sim}{r}_{B2}|\big|)\ \sin\ (\tfrac{\alpha_A+\alpha_B}{2})/(|\underset{\sim}{r}_{A1}|)(|\underset{\sim}{r}_{A2}|)(|\underset{\sim}{r}_{B2}|),$$

where α_A is the angle between $\underset{\sim}{r}_{A1}$ and $\underset{\sim}{r}_{A2}$ and α_B is the angle between $\underset{\sim}{r}_{B1}$ and $\underset{\sim}{r}_{B2}$. The formula is exact if $\alpha_B = \alpha_A$. Although this estimate of misfit dislocation density ignores any relaxation due to elastic strain in the contact layer, its use does enable a comparison with the normal density range of $10^2 - 10^{12}$ dislocations/cm^2 for homogeneous materials. The type of dislocation is unspecified but may be the edge or screw type or a combination of the two.

MATCH1 should be used as a means of ranking possible contact planes in order of the likelihood of a good structural match. This optimizes the more lengthy process of matching contact regions of crystal structures in MATCH2.

The generalized misfit is a measure of the extent to which the pattern repeats (unit meshes) stay near coincidence. Typically, MATCH1 keeps only those networks that require a distance of at least 100 Å before the meshes are out of phase (mesh point of one network halfway between mesh points of the other network). In order to rank a possible contact plane, a measure of the complexity of the associated atomic pattern is needed without actually knowing what the atomic pattern is. The approach used in MATCH1 is to adopt a unit area for a cation and anion, or a molecule, and compare this with the area of the unit mesh of a network to give an estimate of the atomic density. The index actually used is (area of unit mesh in $\text{Å}^2-30\text{Å}^2)/30\text{Å}^2$ where 30Å^2 is taken as the unit area. Thus, meshes with large areas yield higher values of this index. Possible contact planes are sorted on the sum of the generalized misfit and the above index, with those planes having lowest values of the sum ranking highest. These cases will normally be considered first by program MATCH2.

The results of several calculations using MATCH1 are summarized in Table 1. The large number of metric fits, networks whose unit meshes coincide within the limits specified, supports the view the mutual orientation of crystals is controlled by structural analogues. Otherwise, many more orientations would be expected to be observed experimentally.

Table 1

Number of metric fits between $Ca_5(PO_4)_3OH$ and other compounds

$Ca_5(PO_4)_3OH$	16*	$CaCO_3$(a)	297
$Ca_8H_2(PO_4)_6\cdot5H_2O$	11	$CaCO_3$(c)	28
$Ca_4(PO_4)_2O$	82	$BaCa(CO_3)_2$	420
$CaHPO_4\cdot2H_2O$	229†	$Ca(COO)_2\cdot H_2O$	82
$CaHPO_4$	41**	$Ca(COO)_2\cdot2.2H_2O$	18
$Sn_3PO_4F_3$	67	$CaKAsO_4\cdot8H_2O$	132
$CaCO_3\cdot6H_2O$	66	$MgNH_4PO_4\cdot6H_2O$	177

* Possible twinning modes

† Criteria changed to 10%, 4°, 21Å because >1000 matches obtained originally.

** Criteria changed to 15%, 4°, 21Å

Normal criteria:

(i) length mismatch 15% maximum
(ii) inter-vector angle mismatch 10° maximum
(iii) maximum vector length 20 Å

The program MATCH2 carries out the procedure in step 2 of the Introduction. Each of the networks in the matching pairs generated in MATCH1 defines an infinite set of parallel planes in the corresponding compound. To check the gross features of the proposed contact, a preliminary search by the following method is made with the monatomic cations and anions and the central atoms of polyatomic ions, e.g., P in the case of PO_4. Each atom in the structure is allowed to define a specific plane from the infinite set of parallel planes (see Fig. 1). All crystallographically discrete atoms within a predefined distance, typically 0.75 to 1.0Å, of the defined plane are identified. If the resulting slice is sufficiently populated, the immediate environment of each of these atoms is determined and is considered to be that atom's structural motiv (Fig. 2).

All unique interatomic vectors are calculated between members of each motiv. Motivs in the two structures are then compared on the basis of their vector sets so that incremental rotation of the motivs is not necessary at this stage. The comparison includes consideration of vector lengths and the charge product of the two atoms defining each vector. Each vector is used in only one vector match. A figure of merit for the fit of the two vector sets is calculated based on the length misfits of individual vectors and on the percentages of the vector sets matched up. In cases where one motiv encompasses another, the total fit will be good for the smaller and poor for the larger motiv and this possible match will be given a relatively low figure-of-merit.

The inter-vector set figure-of-merit corresponds to a measure of the closeness of fit between these vector sets (see the example in the sample output on p. 49). This in turn is taken as a measure of the similarity of the chemical environments of the central atoms of the motivs. The assay of the chemical environment is necessarily confined here to the ~2Å thick slice through the crystal structure. Thus the environmental similarity of two central atoms, one in compound A and one in compound B, is assessed from the magnitude of the figure-of-merit, and is considered to be directly proportional to this magnitude.

The atoms in compound A are matched one at a time with atoms in compound B in strict order of descending figure-of-merit magnitude (refer to p. 57). The sum of the individual figure-of-merit matches is accumulated to give an overall inter-plane figure-of-merit which, after matching is complete, is divided by the plane area to give an inter-plane figure-of-merit normalized to unit area (p. 57). The normalized inter-plane figure-of-merit may then be used as a quantitative

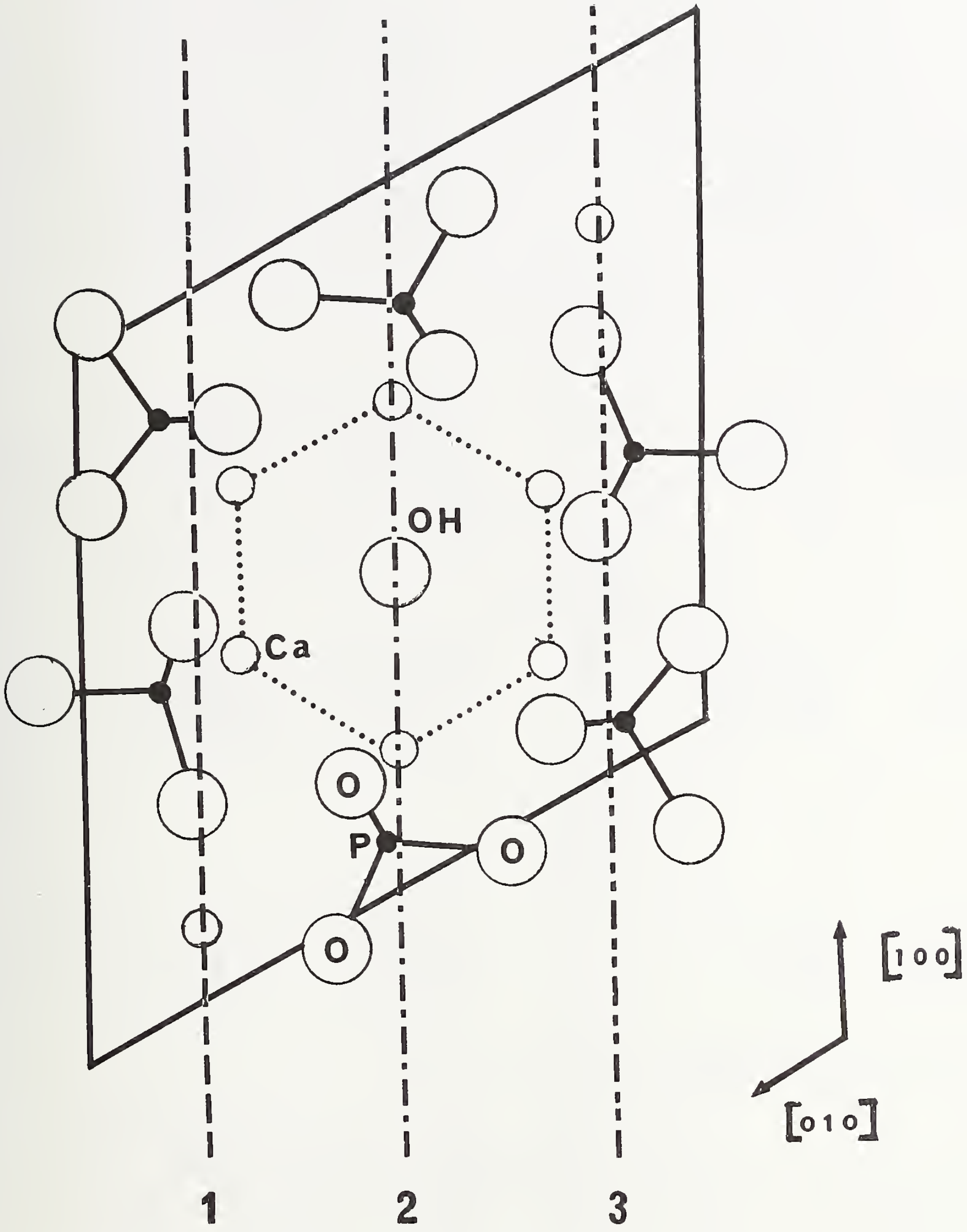


Figure 1. Possible contact planes in $Ca_5(PO_4)_3$ OH.

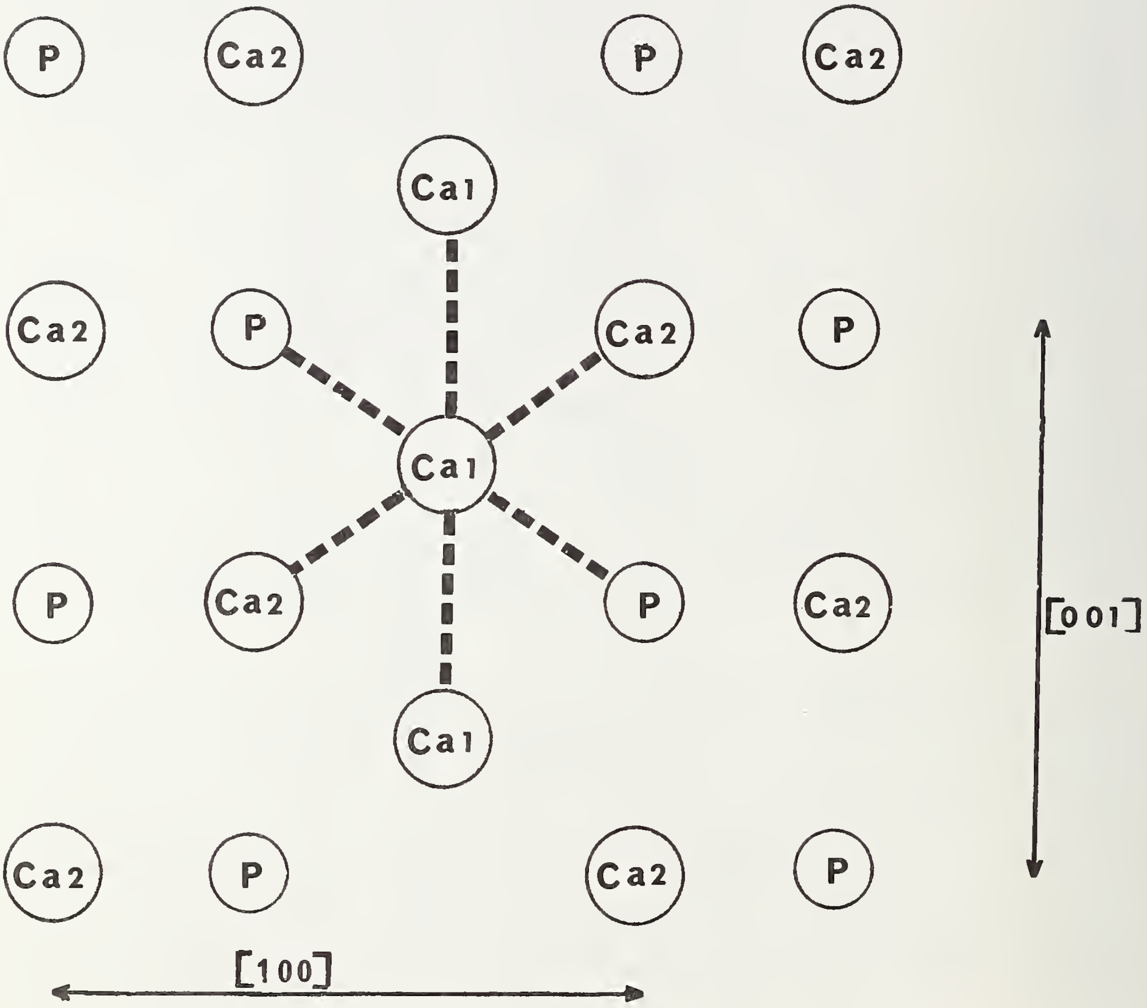


Figure 2. Ca 1 motiv in $Ca_5(PO_4)_3$ OH.

Table 2. Calculated Structural Fits

Slice thickness = 2.00 Å, notiv radius 6Å

A	B	Fit	Net A	Net B	Areas		Atoms	Sort order
HA	HA	9.26	(001,100)	(001,100)	64.8	64.8	$2C_1 2C_2 2P$*; $2C_1 2C_2 2P$	1
		7.96	(100,211)	(100,211)	100.5	100.5	$2C_1 3C_2 3P; 2C_1 3C_2 3P$	3
		7.82	(100,210)	(100,210)	76.8	76.8	$2C_2 3P; 3C_2 3P$	2
HA	OCP	8.32	(001,100)	(001,010)	64.8	64.9	$2C_1 2C_2 2P; C_1 C_2 C_5 P_9 P_{12}$	1
HA	TECP	7.98	(001,100)	(001,010)	64.8	66.4	$2C_1 2C_2 2P; C_5 C_6 C_7 C_8 P_3 P_4$	3
		7.70	(001,100)	(100,001)	64.8	66.4	$2C_1 2C_2 2P; C_1 C_2 C_3 C_4 P_1 P_2$	3
HA	MON	5.84	(001,100)	(100,010)	64.8	45.8	$4C_1 4C_2 4P; 3C_1 3C_2 3P_1 3P_2$	
HA	DCDH	2.85	(002,200)	(010,303)	64.8	96.5	$12C_1 12C_2 6P$; 4C4P	

HA = $Ca_5(PO_4)_3OH$, hydroxyapatite

OCP = $Ca_8H_2(PO_4)_6 \cdot 5H_2O$, octacalcium phosphate

TECP = $Ca_4(PO_4)_2O$, tetracalcium phosphate

MON = $CaHPO_4$, monetite

DCDH = $CaHPO_4 \cdot 2H_2O$, dicalcium phosphate dihydrate

* $2C_1 2C_2 2P$ means that two Ca(1) ions, two Ca(2) ions and 2P atoms as labeled in the reported crystal structure of the material in Column A were found to be in the same slice parallel to the plane defined by the lattice vector given under Net A.

indication of the perfection of chemical fit between two candidates for epitaxy or twinning contact planes, and allows the comparison of all such candidates on a quantitative basis over several compounds. Table 2 provides an overview of the results of several runs of the MATCH2 program. Optionally, MATCH2 also produces a printer plot of the atomic patterns for the contact planes in compounds A and B. The listing of crystal coordinates allows one to label the repeating unit on the plot and visually check that MATCH2 has matched everything properly. See the output example generated by the test deck.

Procedure in MATCH1

The main routine in MATCH1 is element MAIN.

The first card read by element MAIN contains the title of the run, the output unit number, and the ordinal file on the output unit. The output file may be positioned using computer specific routines in subroutine POSITN.

The second card contains the unit cell parameters of the first compound, compound A, from which the reciprocal cell and real cell volume are calculated in subroutine CELL. These quantities are then printed in the listing to allow the input quantities to be checked. The cell of compound B is then read in from card three and treated similarly. The real and reciprocal cell metric tensors are calculated for compounds A and B in subroutine METRIC.

Card four contains the point group number for compound A, the point group number for compound B, the allowed percentage difference on vector lengths, the allowed percentage difference on network angles, and the maximum vector length permitted in the networks. The default options of these last three quantities are 15%, 10°, and 20Å.

The symmetry subroutine SYM which filters out the unique vectors from the triclinic set initially generated by the program, is based on the point group (32 possibilities) underlying the space group of the crystal structure. (Note that the required point group is not necessarily one of the 11 Laue centrosymmetric point groups or related to one of the 14 Bravais Lattices.) Thus all meaningful network matches will have been treated when structural considerations are applied in the subsequent program, MATCH2.

All unique vectors with length less than the maximum value are calculated in the two compounds by generating vector sets in triclinic symmetry and then filtering the sets through the symmetry subroutine SYM. These vectors are sorted into ascending order of length and the resultant values are listed in the output of the program. Vectors in compound A are then matched with vectors in compound B subject to the limitation that the mismatch between vector lengths must be less than the read-in quantity, usually 15%. The resultant vector matches are also output for checking and references purposes.

Networks are generated by taking pairs of vectors in compound A and their matched mates in compound B. The inter-vector angles are calculated in both cases and made less than or equal to 90° by taking the supplement if necessary. Care is taken to use only non-parallel vectors to define networks. Only those cases where these inter-vector angles agree within 10° are accepted for further processing. Subroutine ANGCK rotates the nets to closest coincidence and estimates misfit dislocation density.

Various tests are made throughout the program to insure that the list of network matches does not contain redundancies. At this stage the indices of vectors in new network matches are compared with the indices of vectors in previously obtained matches and complete redundancies removed from the list.

In case the acceptable limits on vectors and network matches are too generous and produce too many matches, the program estimates how much to reduce these criteria to bring the total number of vectors and networks just below their respective maxima of 1000 vectors and 1000 networks in each compound.

Further checks are made to cut down the number of redundancies or near-redundancies. The program takes two networks in compound A and calculates the angle between the normals to the networks. A similar inter-normal angle is also calculated for the network pair in compound B which has previously been tagged as matching the network pair under consideration in compound A. At least one of these two inter-normal angles, one in compound A and the other in compound B, must be greater than 2° for both network matches to survive. Otherwise, the two sets of networks are essentially or actually parallel to one another and the set of networks with the smaller average angle is dropped from the list. The process is repeated until the list of network matches comprises a unique set. At this point the list of networks has been reduced in size as much as is feasible but typically from 10 to 1000 network matches still remain.

To remove the random character of the search when these network matches are input into the structure-matching program MATCH2, the network matches are then sorted in order of probability using quantities calculated with the following criteria in mind:

(1) Corresponding mesh points for the two nets should be as close as possible (i.e., the nets should approach coincidence).

(2) The atomic pattern of the planes should be simple.

The rationale for the second criterion is that the simpler the pattern the higher the probability of its being matched by a similar layer in some other compound. That is, it is easier to match a pattern with few details than one with many details. To put the criteria in (1) and (2) on the same scale by restricting the possible outcomes to the same range, we use the following quantities: (i) 2 RL/(Sum of long diagonals of the nets A and B) where RL is the distance between the corresponding lattice points for net A and net B. (ii) 2RS/ (Sum of short diagonals of the nets A and B) where RS is similar to RL. The theoretical range of these quantities is 0 to 2. These indices yield a measure of how well criterion (1) is being fulfilled.

(iii) $K \cdot \left(\left|\frac{\text{area A}-30}{30}\right| + \left|\frac{\text{area A}-30}{30}\right|\right)$ where we have assigned a unit area of $30Å^2$ as that occupied by a basic structure unit, e.g., one cation and one anion. The range is restricted to 0 to 2 by chosing K, the scale factor. The maximum area allowed is governed by maximum length allowed for a network vector and is typically about $400Å^2$.

The sum of the three quantities (i), (ii) and (iii), is used as a composite sort parameter. Networks with low values of this parameter are considered the most probable candidates for structural matches. In confirmation, our preliminary results have shown that the most important structural matches as determined by MATCH2 in lists of networks which have been sorted using these combined criteria do usually occur in the first three or five members of the list. The sorted list is output on a file, either on magnetic tape or mass storage such as a drum or disc, which can then be transferred to the second part of the matching scheme. An overview of the results of several runs of this program has been given in Table 1, p. 5. Examples of the input and output are given on pages 49 and 50.

Procedure in MATCH2

MATCH2 produces a quantitative estimate of the likelihood of forming polycrystals composed of phases for which the detailed crystal structures are known. The program needs as input (i) the unit cells, symmetry operations and atomic coordinates for the structures under consideration, and (ii) two vector pairs, each pair defining a plane through one of the two crystal structures or two sets of Miller indices. The defined planes may be the result of visual inspection of the crystal structures or may be obtained in a more objective manner as output of the network-match generating program MATCH1.

A slice of predetermined thickness, typically from 1.5Å to 2.0Å, is then taken through each crystal structure. In our studies of calcium phosphates we have found it satisfactory to use only the Ca and P atoms for preliminary surveys to reduce the large number of slices to be considered in greater detail. The set of vectors between atoms in the slice is used to compare atomic arrangements in slices in different compounds and to derive figures of merit for possible epitaxy of the two compounds with the slices under consideration as contact planes.

The flow of the MATCH2 program will now be given in some detail. The main routine is MATCH2 which reads the title of the job from the first card. The unit cell parameters for compound A are read in from the second card and the reciprocal cell and the volume of the real cell are calculated. Next, the symmetry elements followed by the unique set of atoms for compound A are read. Then the program reads the unit cell, symmetry elements, and atoms for compound B. These quantities are immediately output.

The program calculates the real and reciprocal metric tensors for compounds A and B and generates the full cell of atoms. Matrices are calculated to orthogonalize the actual unit cell, to transform from the orthogonal cell back to the actual cell, and to transform the atomic coordinates from their fractional values in the real cell to orthogonal coordinates in Angstroms. The atomic positions and the vectors defining the unit cell edges are transformed to orthogonal angstrom coordinates so that different crystal structures can be compared in the same units and interatomic distances can be calculated efficiently.

At this point the program is ready to read in the first of the networks to be compared from either an intermediate input file prepared by the MATCH1 program or from the card reader. The planes may also be entered in Miller indices. The first read from the intermediate input file if this mode is used is the title of the input file. Then the program enters a loop which begins with the vectors defining the networks being read from the same file.

If an end-of-list signal or a hardware end of file has been read or if the number of reads is greater than the requested maximum value, further calculation is terminated and the program outputs a final summary of inter-slice figures of merit. Otherwise the program then proceeds to check the vectors which define the two networks. First, the indices of each vector are made coprime. If the vectors are read from the card stream rather than an intermediate file, the length of each vector is calculated and the angle between the two vectors defining the network is calculated for each compound. Each angle is made less than or equal to 90° by taking the supplement if necessary. These quantities are already available when the intermediate file is being read. The area of each network is calculated and the ratio of the areas is saved for later scaling of (i) the number of occurrences of each type of atom in the two compounds to a common basis and (ii) the inter-plane figure of merit for this network match to unit area. Similarly, the length of nominally corresponding vectors are compared and the necessary multiples of each length are obtained. The vectors are then scaled by these multiples. In the present program the maximum ratio of these multiples is 4:3.

The program outputs the input as modified by the various decisions that it has made so far. It then calculates and prints the plane normals to the networks and the Miller index designation of the plane defined by the network so that reference may be made to the planes in this convention if desired. When twinning (compound A is the same as compound B) rather than epitaxy is being investigated, the angle between the normal to network A and the normal to network B is calculated and the rotation axis and angle are output to define the twinning mode. The program then calculates for all cases the direction cosines of the plane and the d-spacing. These quantities are written out.

The main program then calls subroutine ATPLAN to determine the populations of all significantly different slices in each crystal structure parallel to the networks specified by the vectors. In subroutine ATPLAN, each atom in turn is allowed to define the central plane of the slice and all the other atoms are checked to see if they are within distance PDIST Å of the plane defined by the first atom, i.e., if they are within the same slice.

Presently the program calculates all possible slices by allowing every atom in the unit cell to define its own slice. Options exist for (i) proceeding with all slices, (ii) removing redundancies based on equal numbers of identically labeled atoms (e.g., Ca 1) or (iii) removing redundancies and subsets.

The variable PDIST must be selected with care. Too large a value will allow several planes to define a particular slice over the one unit cell the program investigates to populate the slice. Too small a value for PDIST may result in some atoms being wrongly excluded from the slice. We have found that an appropriate value is 1.0Å, which, being the distance from the defining plane to the edge of the slice, gives a slice thickness of 2.0Å, i.e., roughly an atomic diameter.

For each atom in a slice, the spacing of the atom from the plane which defines the center of the slice, the ordinal number of the atom which defines the slice and the ordinal number of the atom which is a member of the slice are all stored away in one large array. Only those slices with more than two atoms in them are saved for later use. Subroutine ATPLAN also provides the number of atoms in each slice.

After subroutine ATPLAN has been entered once for each of the two crystal structures being compared, the main program calls subroutine ATVEC to determine the atomic motivs and the vector sets of these motivs. Subroutine ATVEC treats the slices of atoms one at a time. First it determines the number of the occurrences of each kind of atom in the slice as distinguished by the alphanumerical label of each atom. Because the atoms are distinguished by their labels, atoms in different environments (i.e., crystallographically different atoms) must be given different labels, e.g., Ca(1), Ca(2), Ca(3) and so on. This differentiation is necessary to save computing time by finding the motiv for only one Ca(1), Ca(2), etc.

Two methods of calculating the motiv have been investigated. The first is based on the contents of the slice in one unit cell. The problem here is in relating cells of different size. However, the system works very well for cells which are approximately the same size and where one network is not a subset of the other. The second method involves including into the motiv only those atoms which lie within some preconceived distance of the motiv-defining atom. Typically this distance has been 6.0Å, which allows for first and second nearest neighbors. Specifically, the distance was chosen to allow the program to pick out P atoms in both neighboring PO_4 groups in PO_4...Ca...PO_4 chains when the Ca motiv is being constructed and yet not include atoms beyond the first layer of the environment (see Fig. 2). This method is obviously independent of the area of the plane.

In both methods of building up the atom motiv, up to four neighboring unit cells are searched to find those atoms which lie on the plane and which are nearest to the central atom of the motiv, i.e., the motiv definer. Provision is made in both cases for including all atoms with a given alphanumeric label whose distances to the motiv definer are less than 1.25 times the shortest distance from this type of atom to the motiv definer. At the present time, the second method is the one implemented in subroutine ATVEC.

When the motiv has been assembled by considering all the atoms in the slice, the vector set between all atoms within the motiv is calculated as a quantitative description of the motiv. It should be noted that use of the vector set removes any knowledge of the relative orientation of the two patterns to be matched. This is a serious restriction in testing possible cases of twinning where the structure has been rotated or reflected about the normal to a contact plane; in such cases the procedure degenerates into a calculation of the atomic density per unit area. Our planned third stage, MATCH3, will handle these cases and will also act as an extension of MATCH2 for general cases.

The program writes the motiv defining atom, the motiv vector set and several other associated quantities on a temporary mass storage file and then considers the next motiv. At the end of these calculations the program writes an end-of-data flag on the mass storage file and re-enters the subroutine ATVEC to perform similar calculations for compound B. ATVEC can also generate a histogram of various classes of inter-atomic distances on a surface by calling subroutine HISTGM. This feature was added to aid in our studies to develop improved adherents to calcium phosphates.

When control is returned to the main program after the second pass through subroutine ATVEC, the first motiv for each compound is read from the appropriate mass storage files. The number of occurrences of the motiv-defining atom on the plane in each structure is scaled up by the appropriate multiple previously defined by a comparison of the plane areas. The vector sets of the two motivs are then compared. The comparison includes consideration of the charge product of the two atoms which define the ends of the vectors. Thus, charge misfit of greater than 1.5 electrons is at present not permitted in a vector match. Also, vector length misfits greater than 25% are not permitted in matches of individual vectors. After these tests have been made between a vector in the motiv in compound A and all unmatched vectors in compound B, the best fit of length between the vector in compound A and the corresponding one in compound B is tagged as a match and neither of these vectors will be matched again.

After attempts have been made to match all vectors in the two vector sets, the program calculates the percentage vectors matched, the percentage charge mismatch, and the percentage of each vector set matched. If required, the program will at this point output onto an intermediate file the various quantities it has obtained between motiv matches if more than 75% of the vectors in both vector sets are matched and the average mismatch in length or charge is less than 25%.

For all vector sets, an inter-motiv figure-of-merit quantity is calculated based more or less equally on the average distance mismatch and the number of vectors matched. This quantity, which is designed to be 100% for perfect matches, is $[(0.2-T)/0.2]50 + (Z_A + Z_B)/4$, where T, the average mismatch of vectors in A, is compared with 0.2 , and Z_A and Z_B are the percentages of matched vectors in the vector sets of the motivs in compounds A and B. If the two atoms defining the motivs being compared have different charges they are considered to be mismatched chemically. The percentage quantity defining that match is reduced by 20% so that the program will be less likely to match atoms of opposite charge should the vector sets of their motivs accidentally have some correspondence. Such cases are obviously chemically destabilizing.

When an individual figure of merit has been calculated for the possible match of each motiv in compound A with each motiv in compound B, the program attempts in the second half of the MAIN element to match atoms using the inter-motiv figure-of-merit just calculated. The program determined earlier the multiplicative factors which make two plane areas under consideration the same and scaled up the number of atom occurrences in each slice to reflect this. Matching between atoms is accomplished by pairing off the atoms in compound A with atoms in compound B in order of descending value of the inter-motiv figures-of-merit subject only to the number of occurrences of each atom in the slice. Thus, if an atom in compound A has four total appearances and an atom in compound B has only three occurrences and these atoms have a very high matching quotient, the match will be used until the lower number of occurrences is completely satisfied, that is, three times. The fourth match of the atom in compound A must be accomplished by using some other atom in compound B. In general, this procedure works very well and the program is correctly able to identify and match, for example, atoms in cation columns in two compounds.

As the atom-matching proceeds, an accumulative sum is made of the associated inter-motiv figures-of-merit. When all the atomic occurrences in one of the two compounds have been matched, the program calculates an inter-plane figure of merit by dividing the total accumulation of inter-motiv quantities by the maximum of the two network areas to give some idea of matching per unit area.

If the inter-motiv fit is greater than a threshold value initially read from cards (with a default option of 4.0), the option exists of plotting the atomic configuration on the planes in compounds A and B on the line-printer with all plots on a constant scale. The atom labels and positions in the unit cell are listed whether or not the plot option is selected. The plots may be used to resolve ambiguities in matching atoms which have close matches with other atoms.

Ambiguities sometimes exist because an atom in one compound may match two atoms in the other compound within the limits of resolution of this procedure. Because of these ambiguities, a general procedure to assemble matching patterns of atoms in slices by considering individual matches is difficult to program. At present, a general procedure seems unnecessary because visual matching of atoms after reference to the plots and the atom-atom environment fits is quick and provides a chance to check on the validity of the calculations at an opportune stage.

At the end of the assessment of each slice in the structure parallel to a network, the program reads in another network and repeats the procedure. When network read-in is complete, the program outputs the details of up to 20 of the best matches for further consideration. The merit figures may be taken, for example, as implying the likelihood of epitaxy between compounds A and B using the slices as "common material" and the centers of the slices as contact planes. A summary of several calculations of possible epitaxies between $Ca_5(PO_4)_3OH$ and some other calcium phosphates is given in Table 2, p. 9 Examples of the input and output are given on pages 51 and 52.

Algorithm for MATCH1

Comments refer to operations carried out in the subroutines named in capital letters or otherwise to operations carried out in the main program MAIN .

```
Start:  MAIN    (Main program)

        Initialize

        Position output file in POSITN

        Write title on output file

        Read cell of A in CELL

        Read cell of B in CELL

        Calculate real and reciprocal metric
        tensors for A and B in METRIC

        Read boundary conditions and initialize
        them if required

        Calculate lattice vector lengths for A and
        B in DVCALC

        Sort lattice vectors into order of increasing
        length in SORT

        Output lattice vector lists for A and B

        Find vector matches in terms of lengths
        between lattice vector set in A and B

        Take two vectors at a time in A to generate
        network, calculate inter-vector angle.  Do
        same for B
```

Compare inter-vector angles in A and B, save inter-network match if angles are within prescribed limits

Remove redundancies in the form of parallel or nearly parallel networks

Sort networks into list based on aggregated criterion which in turn is based on misfits of vector lengths and angles and on area of plane. Write sorted list on output file for transmission to MATCH2 program

General purpose of subroutines in MATCH1

ANGCK

Calculate the network angle for compounds A and B. Find asimuthal angle to place nets to closest coincidence.

CELL

Read the real cell, calculate the real cell volume and the reciprocal cell.

COMPAR

Compare two lattice vectors for identity of components.

CHECK

Entry in COMPAR. See if two sets of vectors have equivalent indices.

CROSS

Vector cross product routine for triclinic cells. The resulting vector is the same type as the input vectors (co- or contra-variant) and is not normalized.

DVCALC

Generate the unique set of vectors for a point group, using subroutine SYM. Calculate the vector lengths via DIST.

MAIN

Main program. Reads cells, calculates unique vectors, matches vectors in A and B in terms of their lengths, takes vectors in each compound in pairs to generate networks, checks intervector angle matches in A and B, removes redundancies and near-parallel cases.

HKLGEN

Unpack indices of lattice vector from packed word.

METRIC

Calculate metric tensor from cell dimensions.

MV

Multiply vector by matrix.

PLANEQ

Find Miller index representation of network defined by two real cell lattice vectors.

POSITN

File positioning routine. Dummy routine at present.

SORT

Sort input quantities into ascending order.

SYM

Reduce vector to unique form as determined by point group. Eliminates redundant vectors.

TEST

Governs the overall checking of whether two networks are the same based solely on indices.

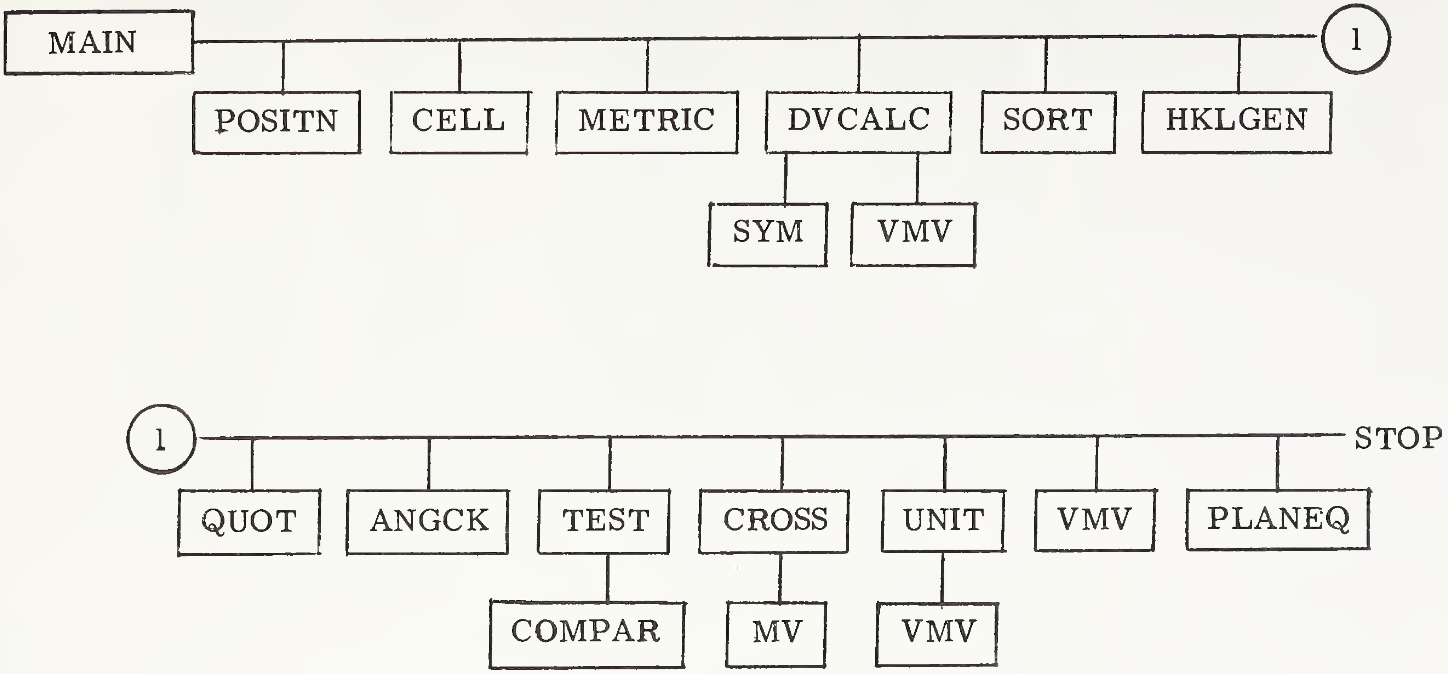
UNIT

Make input vector into unit vector.

VMV

Generate scaler product for input vector when given the appropriate metric tensor.

Hierarchy of subroutines in MATCH1



Main variables in MATCH1

COMMON /STORE/BUFF (1000,32)

The BUFF array is used to save space by overlaying variable lists in core.

Those variables in the following list which have A as one of the initial two or final two characters are quantities related to compound A, one of the two compounds under consideration. In the variables related to compound B, the A is replaced by B. Only the A variables are mentioned below.

A, RA	Real and reciprocal cell parameters for A.
AM, RA	Real and reciprocal metric tensors for A.
AREAA	Area of plane defined by the two A vectors referenced in the corresponding element of the MATCHA array.
ANGAS	Angle for A network saved in corresponding member of MATCHA array.
DELTAD	Fractional mismatch in length of lattice vectors matched up in corresponding element of MATCH array. The corresponding element of MATCH contains the packed ordinal numbers of the paired vectors.
JKLA	Array of packed indices of lattice vectors. The indices are multiples of the cell edges.
MATCH	Packed ordinal numbers of vectors matching in lengths within prescribed criterion. One vector belongs to compound A and the other to compound B.
MATCHA	Array derived from packing two MATCH numbers, making a total of four ordinal numbers of vectors packed together. The four vectors define two matched networks.

Algorithm for MATCH2

Comments refer to operations carried out in the subroutine name in capital letters or otherwise to operations carried out in the main program, MAIN.

The card input to the program is described on page 39.

```
Start: MAIN  (Main program)

       Initiallize

       Read cell A in CELL

       Read symmetry elements A in SYMIN

       Read atoms for A in ATOMIN

       Read cell for B in CELL

       Read symmetry elements B in SYMIN

       Read atoms for B in ATOMIN

       Output input quantities in OUTP
```

Calculate real and reciprocal metric tensors for A and B in METRIC

Generate full cell of atoms for A and B in ATCELL

Calculate orthogonization matrices for cells in ORTH

Read in plane defining information, either as plane normal in intercept notation (generate lattice vectors notation in VECTS) or as lattice vectors defining a network in real cell lattice (generate intercept notation in PLANEQ)

Compare vector lengths

Scale up vectors so that plane areas are equivalent

Find plane normals in VNORM

For network notation in input, find intercept notation in PLANEQ

For twinning, calculate twin axis via VNORM and rotation angle.

Calculate direction cosines and d-spacings via MV and VMV.

Output intercept notation, twinning information, direction cosines and d-spacings where appropriate

Calculate perpendicular spacing of atoms from plane in compound A in ATPLAN

Ditto for B in ATPLAN

Calculate atomic motiv and motiv vector sets for compound A in ATVEC, store results on temporary file NDRUMA, print contents of motivs if required, calculate histograms of distances in structural layer (histograms separated according to charge of atoms) in HISTGM if desired.

Ditto for compound B in ATVEC and NDRUMB

Read information for one motiv at a time from temporary files and begin motiv-motiv comparison

Scale up atom occurrence count for disparity in plane areas

Compare vector sets of each motiv in compound A with each motiv in compound B

Optional output of motiv-motiv match parameters on saved file

Count up preliminary merit indicators

Calculate inter-motiv figure-of-merit

Calculate inter-plane figure-of-merit based on best individual atomic matches, i.e., inter-motiv figure-of-merit, and scale to unit area

Optional plot of atoms in layer

Optional listing of positional parameters of atoms in layer

Store up to twenty best inter-plane fits, as revealed by the highest magnitudes of the inter-plane figures-of-merit

Read another vector set, or at conclusion of job, output up to twenty best matches

General purpose of subroutines in MATCH2

ATCELL

Expand the asymmetric unit of atoms into the full cell.

ATOMIN

Read atom list into array ATOM. There are N atoms total. List terminated by end-of-file card.

ATPLAN

Take each atom in turn as a plane definer and find all those atoms in the rest of the unit cell which are within distance PDIST (typically 1Å) of that plane.

ATVEC

Find the environment on the plane (i.e., the motiv) for each crystallographically different atom (as designated by the atom name, e.g., Ca 1, Ca 2, etc.). Also count up the number of times each atom appears in the slice and calculate the motiv for one appearance only. Include in the motiv only those atoms which are closer than "CRITD", initiallized at 6Å, and which are within the factor "TESTDM", initiallized at 1.25, of the closest distance for that type (e.g., Ca 1) of atom. Calculate the vector set of the motiv, remove any redundancies and write the results on a scratch file. Optionally list the identity and position of each member of each motiv and optionally call HISTGM to generate histograms of distances.

CELL

Read the real cell, calculate the real cell volume and the reciprocal cell.

CONSOL

Subroutine to incorporate a list of new atoms into a list of old atoms and remove redundancies.

COPRIM

Make coordinates of vector coprime, considering a maximum highest common factor of 4.

CROSS

Vector cross product routine for triclinic cells. The resulting vector is the same type as the input vectors (co- or contra-variant) and is not normalized.

HISTGM

Use vector lengths and charge product of atoms at ends of vector to generate histograms based on the interatomic distances between various kinds of atoms.

MAIN

Main program, sets up initial quantities, reads initial input, reads vector sets, matches vector sets of motiv, picks out atom-to-atom correspondence between compounds A and B and saves up to the 20 best inter-plane matches.

MI3

Matrix inversion subroutine for 3 by 3 matrix.

METRIC

Calculate metric tensor from cell dimensions.

MV

Matrix multiplying vector.

ORTH

Calculate matrix to orthogonalize triclinic cell and transform positions with coordinates in fractions of the cell edges to coordinates in orthogonal angstroms.

Orientation:

X parallel to (bXc)

Y parallel to cX(bXc)

Z parallel to c

OUTP

List the cell, symmetry elements and atomic positions read in.

PLANEQ

Find Miller index representation of network defined by two real cell lattice vectors.

PLOTLF

NBS utility routine to plot on a fixed scale on line printer. Maximum and minimum values along x and y are user-specified.

POS

Put atom back in unit cell if it is outside. Consider one axis per call.

POSITN

Position tape file to file specified using code compatible with computer. Dummy routine at present.

PROJT

Rotate atomic coordinates (in orthogonal angstroms) of atoms on plane so that these atoms lie in the *xy* plane. Used as a precursor to plotting.

QUOT

Compare A and B by calculating max (A,B)/min (A,B). Set equal to 10^6 if min (A,B) equals zero.

SYMIN

Read symmetry elements.

TRANSF

List atoms in plot with coordinates as fractions of real cell axes, provide key between atom identity and alphabetic symbol used in plot. Call PLOTLF to generate plot on line printer.

TRORTH

Transform entire atom list from fractional coordinates to orthogonal angstroms.

UNIT

Make vector into unit vector.

VECTS

Transform plane normal notation into lattice vector notation, prepare for later d-spacing calculation from vector notation.

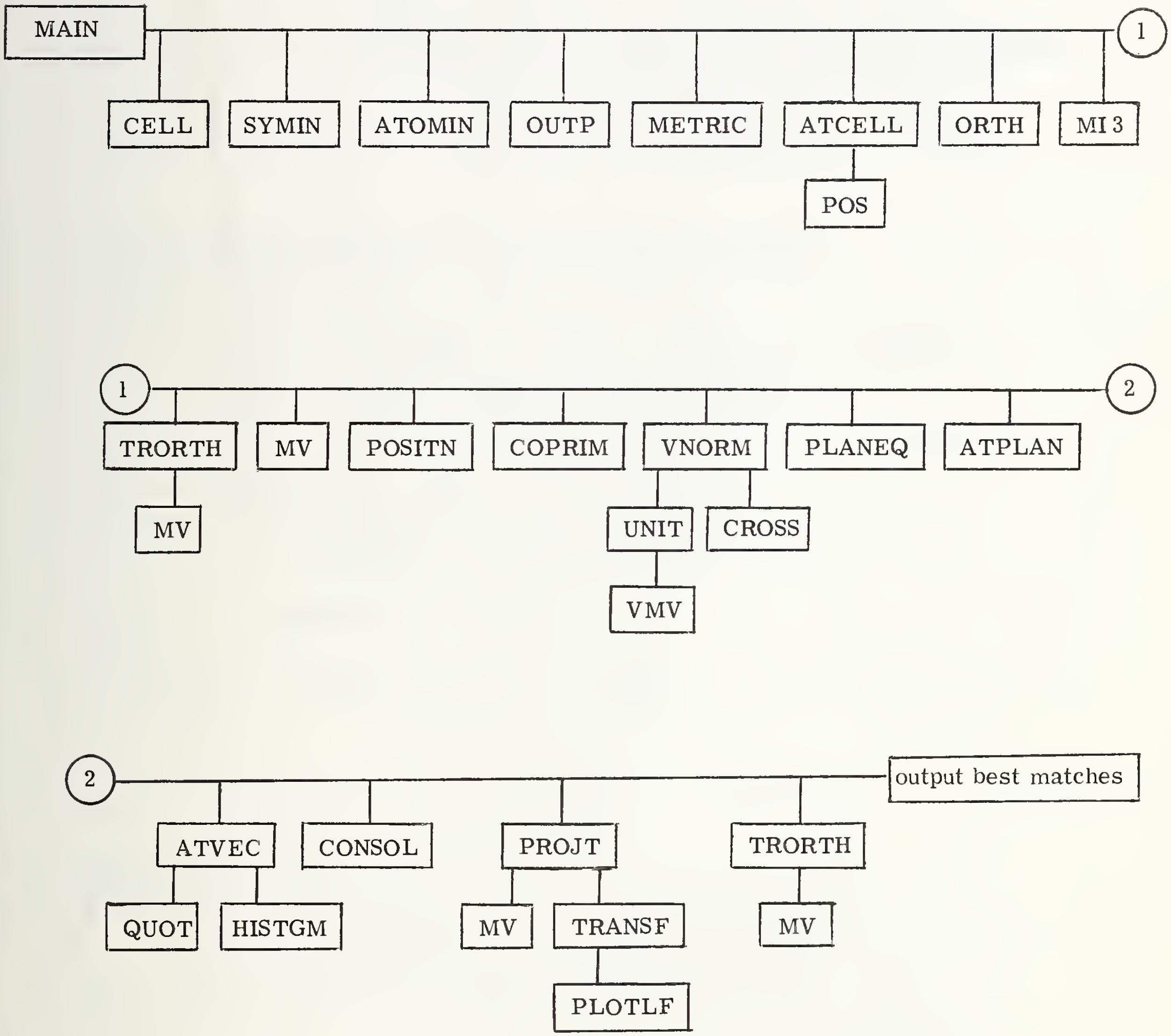
VMV

Calculate bilinear or quadratic form, e.g., scaler product of two vectors.

VNORM

Take two vectors with coordinates given as fractions of cell edge and calculate the normal to these two vectors in the same coordinates.

Hierarchy of subroutines in MATCH 2



Main variables in MATCH2 (initiallized values in parentheses)

COMMON/IN/IN,NOUT

IN - Logical unit for card reader (5)

NOUT - Logical unit for lister (6)

COMMON/PLANE/PDIST, PDIST2, CRITD, TESTDM

PDIST - Distance out from central plane to edges of slice through structure (1.0Å).

PDIST2 - Distance from central plane inside which atoms will lie if the surface is fairly smooth. Used as roughness gauge.

CRITD - Distance to go out from an atom in collecting neighbors to use in assembling the atom's motiv (6.0Å).

TESTDM- Ratio of largest interatomic distance to smallest interatomic allowed in considering chemically equivalent atoms for inclusion in motiv (1.25).

PARAMETER* statement for dimensioned variables

```
NDIM1  =  100, NDIM2  =  1000, NDIM3  =   50,
NDIM4  =   50, NDIM5  =   500, NDIM6  = 5000,
NDIM7  =   20, NDIM8  =   100.
```

Important dimensioned variables in MATCH2

Variables with 'A' as one of the first two or last two characters are associated with compound A, and their meanings are listed below. Variables with B replacing A in a compound A name are associated with compound B but have not been listed below. Minor variables have also not been listed.

---

* Univac 1100 series FORTRAN V Program Reference Manual UP4060 Revision II (1973).

A(6) - Real cell of A.

AM(3,3)- Real metric tensor for A.

ATA(3) - Orthogonal coordinates of 1,0,0 point in A.

ATB(3) - Orthogonal coordinates of 0,1,0 point.

ATC(3), BTA(3), BTB(3), BTC(3) - Similar quantities.

ATNEWA (NDIM5,5) - Used mainly in ATVEC to store the atoms in each atomic motiv.

ATOMA (NDIM1,5) - Atom name, coordinates and charge for A.

FA (NDIM2), IA (NDIM2), equivalenced arrays. First member is perpendicular spacing in floating point of atom in slice in A from plane in center of slice. Second member is atom ordinal number of plane definer, and third member is atom ordinal number of atom whose spacing from plane is first member. Repeats for each atom in slice. Starts with plane defining atom.

KTA (NDIM4) - Number of occurrences in slice of crystallographically different atoms. Given once for first occurrence of atom in list.

MATCHA (NDIM4) - Number of matches each atom has been assigned to during matching of atoms in A with atoms in B via inter-motiv figures merit.

NTOTA (NDIM3) - Array containing the number of atoms on each plane.

NVECTA (NDIM6)- Array which is 0 if vector in set B presently unmatched by one in set A, 1 if vector has been matched. Used in vector set comparison.

PLANEA(3) - Direction cosines of network plane in A.

PLANEC(3) - Lattice vector coordinates of normal to network plane in A (initially intercepts if plane read in this notation rather than as lattice vectors).

PLANEB(3), PLANED(3) - Similar quantities for B.

PLANEF(3) - Rotation axis of twinning operation considered.

QUANT(NDIM4,NDIM4) - Inter-motiv figures of merit calculated from misfit of vector sets of atom motivs.

RA(6) - Reciprocal cell for A.

RAM(3,3) - Reciprocal metric tensor for A.

TA(3,3) - Orthogonalization matrix for unit cell of A.

SYMA(24,12) - Symmetry elements for A.

TAINV (3,3) - Matrix to transform orthogonal cell to actual cell.

VECA1(3), VECA2(3), VECB1(3), VECB2(3) - Vectors defining plane in compounds A and B respectively.

VECTA (NDIM6,2) - Length of vector in motiv and charge product of atoms at end of vector.

Card input to MATCH1

(An example is given on page 48).

Card 1 Output unit, file, title (Read in main routine)

FORMAT (2I2,12A6)

Col.	
2	Logical unit number for output tape. Greater than 6 if output on tape required.
4	Output file number if output tape specified.
5-76	Title

Card 2 X-RAY-type* cell card for compound A, read in subroutine CELL

FORMAT (A4,2X,A6,1X, 3F8.4, 3F9.5)

Col.	
1-4	CELL
7-12	Compound Identification
14-21	a. cell dimension in angstroms
22-29	b. cell dimension
30-37	c. cell dimension
38-46	cos alpha or alpha in degrees
47-55	cos beta or beta in degrees
56-64	cos gamma or gamma in degrees

Card 3 X-RAY-type cell card for compound B, read in subroutine CELL

Card 4 Boundary conditions, read in MATCH1

FORMAT (A6,4X,2I5,3F10.0)

Col.	
1-6	CONTRL
15	NSYMA, point group number compound A. See International Tables for X-ray Crystallography, The Kynich Press (Birmingham, England) Vol. 1, Table 3.3.2. Count as follows: 1 is #1, 1-bar is #2, 2 is #3, etc.

---

* The X-RAY system of crystallographic programs, J. M. Stewart, G. J. Kruger, H. L. Ammon, C. Dickinson, and S. R. Hall, Technical Report TR-192, University of Maryland, College Park, Maryland, June 1972.

Col.	20	NSYMB, ditto for compound B.
	21-30	TESTD, fractional maximum mismatch allowed in judging goodness of match of two vectors, one from compound A and one from compound B. Set equal to 0.15 if left blank.
	31-40	TESTA, maximum mismatch in degrees of the angles in the nets in compounds A and B. Set equal to 10 if left blank.
	41-50	DMAX. Maximum length of a vector used in net definition. Set equal to 20 angstroms if left blank.
	51-55	NTEMP. Flag for future use.
	56-60	NTWIN. Set to one for twin calculation.
	61-65	FMULT. Multiplier of TESTD to provide cutoff for sort key. If less than 1.0, program sets it to 1.0.

Card Input to MATCH2

(An example is given on page 51)

Card 1 FORMAT (12A6) (Read in main routine)

Col. 1-72 Any title

Card 2 Input/output files, layer thickness, motiv radius, mismatch criteria (read in main routine)

FORMAT (A6,7I2,4I1, 1X, 5F5.0, 1X, A4, F5.0, 5I5)

Col.	
1-6	CONTRL
8	Logical number of input unit. Input can be from output of MATCH1 program or from cards.
10	Actual file on this unit (zero leaves unit untouched before data are read off it).
12	Output unit if information saved on file as well as printed.
14	File number on output file.
16	Number of records to skip on input file before beginning calculations (to allow continuation of job curtailed by maximum time, etc.).
18	Number of records to read before stopping. Set equal to 5 if left blank.
20	0: No output of atoms in slices, keep all redundancies (2 or 3 recommended). 1: Write out atoms in slice, keep all redundancies.

2: Write out atoms in slices, remove all redundancies (i.e., same number of atoms with particular alphanumeric labels in each slice).

3: Write out atoms in slices, remove redundancies and subsets of other slices.

4: Write out checking information in motiv-building subroutine ATVEC.

Col. 21	Positive number if summary information punched on cards for later sorting.*
22	Positive number if Miller indices rather than network vectors read in.
23	Positive number if histograms of surface vectors to be generated. (Check subroutine HISTGM for how this is unraveled from list of vectors and associated charge products.) If the number is 2, the program outputs only the histograms and does not calculate any atom matches. It also punches the histogram information on cards.
24	Positive number if this is a twinning calculation, program then calculates the general rotation between the matching networks.
26-30	Half of slice thickness desired, i.e., distance out from plane defining the center of the compositional plane in the crystal to the edge of the slice common to the structures involved in epitaxy. Set equal to 1.0 angstroms if left blank.
31-35	Inner portion of slice thickness. Set equal to 0.75 angstroms if left blank. Used to count up atoms in "fringe areas" of slice and to measure how uneven that surface of the crystal would be.

* See p. 46 for description of card output.

Col. 36-40	The radius inside which all members of an atom motiv must fall. Set equal to 6.0 angstroms if left blank.
41-45	The maximum divergence of distances from identical atoms in the environment to a motiv defining atom for both atoms in the environment to be included in the motiv. Set equal to 1.25 if left blank. This is a divergence factor, i.e., the maximum distance allowed is 1.25 times the minimum distance found.
46-50	The maximum fractional mismatch in length allowed between vectors in different motivs if these vectors are to be considered as a possible match (the best match of all is the one actually taken, but the number of vectors left unmatched is an important parameter in the program). Set equal to 0.15 if left blank.
52-55	ID for any punched card output.
56-60	Minimum merit figure (blank = 4.0) for output of surface atom coordinates in numerical form.
61-65	Positive number for lister plots of surface atoms.

Col.	66-70	Positive number if output of motiv contents required. (This is usually a good idea so you can see what is being perpetrated in your name or at least your account. It also allows you to assess the efficacy of your chosen motiv radius.)
	71-75	Initial slice number for compound A (for continuation of previous calculation). May be left blank.
	76-80	Initial slice number for compound B. May be left blank.

Card 3 Cell card in X-RAY-type* format, read in subroutine CELL

FORMAT (A4,2X,A6,1X3F8.4,3F9.5)

Col.	1-4	CELL
	7-12	Compound identification
	14-21	cell dimension
	22-29	cell dimension
	30-37	cell dimension
	38-46	cos alpha or alpha in degrees
	47-55	cos beta or beta in degrees
	56-64	cos gamma or gamma in degrees

---

* See p. 37.

Card 4 Symmetry elements in ORTEP[†] format, (read in subroutine SYMIN).
FORMAT (1X,F14.10,3F3.0,2(F15.10,3F3.0)) with sentinel in Column 1 on last card.

Col.	
2-15	Translation for 1st atomic coordinate.
16-18	X
19-21	Y
22-24	Z
	1 for X, 2 for Y, 3 for Z used in first atomic coordinate with sign.
25-39	Translation for second atomic coordinate.
40-42	X
43-45	Y
46-48	Z
	1 for X, 2 for Y, 3 for Z used in second atomic coordinate with sign.
49-63	Translation for third atomic coordinate.
64-66	X
67-69	Y
70-72	Z
	1 for X, 2 for Y, 3 for Z used in third atomic coordinate with sign.

[†] ORTEP: A FORTRAN thermal-ellipsoid plot program for crystal structure illustrations. C. K. Johnson, ORNL-3794 (Revised), Oak Ridge National Laboratory, Oak Ridge, Tenn., June 1965.

Card 5 Atoms in XRAY-type * format (read in subroutine ATOMIN)

FORMAT (7XA6, 3F8.5, F5.2)

Col.	8-9	Atom type, e.g., Ca. Make sure each atom has a unique designation such as Ca 1, Ca 2, etc.
	12-13	Number of atom.
	14-21	X fractional coordinate.
	22-29	Y fractional coordinate.
	30-37	Z fractional coordinate.
	38-42	Charge

After last atom card include appropriate end of file card as end of atom list signal.

Repeat cards 3, 4 and 5 for second compound.

---

* See p. 37.

Card 6 Vector indices or Miller indices if any of this information read from cards (read in MAIN).

FORMAT (3I4) for vectors or (3F4.0) for intercepts

Col.	4	u for first vector in first compound or Miller index h.
	8	v for first vector in first compound or k.
	12	w for first vector in first compound or ℓ

Repeat for second vector in first compound, and then for first and second vectors in second compound.

Miller index notation requires one card per plane per compound.

Input always terminated by EOF card so program goes to prepare summary of the results for the current run.

Optional Summary Output On Punched Cards

Summary information on punched cards may be obtained by placing any positive number in Column 21 of the MATCH2 control card, card 2.

Cards from runs through different parts of the intermediate file of metric matches as produced by MATCH1 or from several cases may be combined and sorted for an overall view. The cards contain the following information:

Col. 1-3	ordinal number of A slice
4-6	ordinal number of B slice
7-9	ordinal number of network match
10-12	ordinal of this card in this output
13-18	overall merit figure
19-23	fractional mismatch of first vector in A and B
24-28	fractional mismatch of second vector in A and B
29-33	fractional mismatch of angles in A and B
34-35	u for first vector in A
36-37	v for first vector in A
38-39	w for first vector in A
40-41	u for second vector in A
42-43	v for second vector in A
44-45	w for second vector in A
46-47	u for first vector in B
48-49	v for first vector in B
50-51	w for first vector in B
52-53	u for second vector in B
54-55	v for second vector in B
56-57	w for second vector in B
58-64	estimate of dislocation density
65-66	h of Miller notation of plane in A
67-68	k of Miller notation of plane in A
69-70	ℓ of Miller notation of plane in A
71-72	h of Miller notation of plane in B
73-74	k of Miller notation of plane in B
75-76	ℓ of Miller notation of plane in B
77-80	card ID

Computer Requirements

MATCH1: At least $28{,}000_{10}$ words on an intermediate scratch file (tape or mass storage such as disc or drum).

9200_{10} words of core for instructions and $27{,}700_{10}$ for data. Optional output on binary file for transfer to MATCH2.

MATCH2: About $35{,}000_{10}$ words on each of two intermediate scratch files.

$9{,}800_{10}$ words of core for the instructions and $49{,}050_{10}$ for data. Optional output of good matches on binary file.

Both programs pack vector indices or ordinal numbers of related array elements into one word. A computer word length of at least 36 bits is necessary for this procedure to be reliable.

MATCH1. TESTDECK

```
 8   TEST  DECK  FOR  MATCH1
CELL     HA      9.4151    9.4151    6.8810                        -.50000
CELL     OCP     19.661     9.509    6.822      90.17      92.34      108.41
CONTRL          23      2
```

```
     TEST DECK FOR MATCH1

OUTPUT DN UNIT   8 FILE   0 IF UNIT NUMBER IS LESS THAN 7,THERE WILL BE NO SUCH OUTPUT

REAL CELL FDR CDMPOUND A IS  9.4151  9.4151  6.8810    .0C0    .000   -.500

  RECIPRDCAL CELL IS  .12264  .12264  .14533  .00C00  .00000  .50000

REAL CELL FDR CDMPDUND B IS 19.6610  9.5090  6.8220   -.C03   -.041   -.316

  RECIPRCCAL CELL IS  .05366  .11085  .14673  .01674  .04402  .31621

 PDINT  GROUPS  ARE ,  23 AND   2
  THE DISTANCES  IN DIFFERENT CRYSTALS MUST AGREE WITHIN   .15*100 PERCENT
   THE ANGLES MUST AGREE WITHIN 10.0C DEGREES, AND ALL DISTANCES MUST BE LESS THAN 20.00ANGSTROMS


DISTANCES,INDICES AND ORDINAL NUMBER FOR CDMPDUND A
    6.88   0   0   1   1
    9.42   1   0   0   2
   11.66   1   C   1   3
   13.76   0   0   2   4
   16.31   2   1   0   5
   16.67   1   0   2   6
   17.70   2   1   1   7
   18.83   2   C   0   8


DISTANCES,INDICES AND ORDINAL NUMBERS FOR CDMPOUND B
    6.82   0   0   1   1
    9.51   0   1   0   2
    9.51   0  -1   0   3
   11.69   0   1   1   4
   11.72   0  -1   1   5
   13.64   C   C   2   6
   16.61   0   1   2   7
   16.65   0  -1   2   8
   18.94   1   1   0   9
   18.94  -1  -1   0  10
   19.02   0   2   0  11
   19.02   0  -2   0  12
   19.66   1   0   0  13
   19.66  -1   0   0  14
   19.85   1   1   1  15

        34 MATCHING VECTORS FDUND FDR TESTD =  .150

MATCHES FOUND BETWEEN VECTORS-(ORDINAL NUMBER OF VECTOR OF FIRST CDMPDUND)*1000 + (ORDINAL NUMBER OF SECOND COMPOUND)

     1001      2002      2003      3004      3005      4006      5007      5008      5009      5010      6007      6008
     6009      6010      6011      6012      7007      7008      7009      7010      7011      7012      7013      7014
     7015      8007      8008      8009      8010      8011      8012      8013      8014      8015
```

```
 THE  561 NETWDRKS DBTAINABLE BY PAIRING THE VECTOR  MATCHES GIVEN ABDVE REPRESENT PDSSIBLE CONTACT PLANES.
THESE NETWDRKS ( ONE IN COMPDUND A AND DNE IN COMPDUND B ) ARE  SUBJECTED TO THE FOLLDWING TESTS:

1. THE ANGLES BETWEEN THE NETWORK SIDES MUST BE GREATER THAN TWD DEGREES FDR BDTH COMPDUNDS.

2. THE DIFFERENCE BETWEEN THE NETWORK ANGLES IN CDMPDUND A  AND IN CDMPOUND B MUST BE LESS THAN 10.00 DEGREES.

3. THE AZMIUTHAL ANGLE IS CALCULATED  WHICH PLACES  THE NETS IN CLDSEST CDINCIDENCE . MATCHES ARE DESCARDED WHEN THE RESULTING
DISPLACEMENTS DF THE CORRESPONDING LATTICE  PDINTS FOR BDTH COMPOUNDS ARE SO MERGED THAT THE ESTIMATED MISFIT DISLDCATION
DENSITY IS GREATER THAN 10**12/CM**2.

4. ALL NEW NETWDRKS ARE CHECKED AGAINST  PREVIDUSLY STORED ONES TO ELIMINATE REDUNDANCIES.
IF 2 NETWDRK MATCHES ARE WITHIN 2 DEGREES DF BEING PARALLEL. THE MATCH WITH THE SMALLER AREA (DR,IF THE AREAS ARE EQUAL.THE
LARGER ANGLE) IS RETAINED PRDVIDED THE SDRT KEYS AGREE WITH IN 10 PERCENT. DTHERWISE, THE MATCH WITH THE SMALLER SDRT KEY
IS SAVED.



          IN THE FOLLDWING COLUMNS
          DA1= LENGTH OF VECTOR 1 DEFINING NETWDRK IN COMPOUND A
          DB1= LENGTH DF VECTDR 1 DEFINING NETWORK IN CDMPOUND B
          DA2= LENGTH DF VECTDR 2 DEFINING NETWORK IN CDMPOUND A
          DB2= LENGTH DF VECTOR 2 DEFINING NETWORK IN COMPOUND B
          ANGA= ANGLE IN NETWORK IN COMPOUND A(BETWEEN DA1 AND DA2)
          ANGB= ANGLE IN NETWDRK IN COMPDUND B(BETWEEN DB1 AND DB2)
          (1)= FRACTIDNAL MISMATCH DF LDNG NETWDRK DIAGDNALS DF A & B
          (2)= FRACTIONAL MISMATCH OF SHDRT NETWORK DIAGONAL DF A & B
          (3)= AZMIUTHAL ANGLE RELATING SHORT SIDES OF NETS A AND B
          (4)= ABS((AREAA-30.)/30.)+ABS((AREAB-30.)/30.)
          (5)= SORT KEY = (1)+(2)+(4)
          (6)= AREA OF NETWORK IN COMPOUND A
          (7)= AREA OF NETWDRK IN COMPOUND B
          (8)= SEQUENCE NUMBER IN LIST DF SORTED NETWORK MATCHES
          SECOND LINE UNDER VECTORS= MILLER INDICES FCR NETWORK PLANE
          SECOND LINE UNDER (1).(2) = INTERFACIAL DISLOCATIONS /CM**2 ASSUMING NO ELASTIC STRAIN

  DA1    DB1   DA2   DB2    ANGA    ANGB       VECTOR SET 1           VECTDR SET 2       (1)  (2)   (3)  (4)  (5)    (6)    (7)  (8)
 6.88   6.82  9.42  9.51   90.00   89.83 (  0  0  1,  1  0  0) (  0  0  1,  0  1  0) .010 .009   .11 .014 .033   64.8   64.9    1
                                         (    0    1    0)     (    1    0    0)          .132+11

 6.88   6.82 18.83 18.94   90.00   87.49 (  0  0  1,  2  0  0) (  0  0  1,  1  1  0) .019 .011  1.66 .040 .070 129.6 129.1    2
                                         (    0    1    0)     (   -1    1    0)          .402+10

 6.88   6.82 18.83 19.66   90.00   87.66 (  0  0  1,  2  0  0) (  0  0  1,  1  0  0) .052 .030   .20 .041 .123 129.6 134.0    3
                                         (    0    1    0)     (    0    1    0)          .282+11


          3 UNIQUE MATCHES FOUND WITH SDRT KEY VALUES LESS THAN .150

       37 DTHERWISE ACCEPTABLE NETWORK MATCHES DISCARDED BECAUSE THEY WERE WITHIN 2 DEGREES OF BEING PARALLEL
TO RETAINED NETWORK MATCHES

THIS JDB COMPLETE
```

MATCH2. TESTDK

```
      HA/OCP   MATCH LAYERS
CONTRL 5 0 0 0 0 0 3 000                                                   1    1
CELL    HA      9.4151  9.4151  6.8810                            -.50000
               .00 -1  0  0              .00  0 -1  0                  .00  0  0 -1
               .00  1  0  0              .00  0  1  0                  .00  0  0  1
               .00 -1  0  0              .00  0 -1  0                  .50  0  0  1
               .00  1  0  0              .00  0  1  0                  .50  0  0 -1
               .00  0 -1  0              .00  1 -1  0                  .00  0  0  1
               .00  0  1  0              .00 -1  1  0                  .50  0  0  1
               .00  0  1  0              .00 -1  1  0                  .00  0  0 -1
               .00  0 -1  0              .00  1 -1  0                  .50  0  0 -1
               .00 -1  1  0              .00 -1  0  0                  .00  0  0  1
               .00  1 -1  0              .00  1  0  0                  .00  0  0 -1
               .00  1 -1  0              .00  1  0  0                  .50  0  0  1
1              .00 -1  1  0              .00 -1  0  0                  .50  0  0 -1
ATOM    CA     1  .3333  .6667   .0014    2.
ATOM    CA     2  .2467  .9933   .2500    2.
ATOM    P         .3985  .3684   .2500    -1.
@EOF
CELL    OCP     19.661   9.509   6.822   90.17    92.34   108.41
              0.00  1  0  0             0.00  0  1  0                 0.00  0  0  1
1             0.00 -1  0  0             0.00  0 -1  0                 0.00  0  0 -1
ATOM    CA    1    .0720   .7941   .0055  2.
ATOM    CA    2    .0706   .8058   .5037  2.
ATOM    CA    3    .3665   .0310   .0234  2.
ATOM    CA    4    .3631   .8353   .5339  2.
ATOM    CA    5    .1073   .4499   .7626  2.
ATOM    CA    6    .2012   .6601   .2757  2.
ATOM    CA    7    .2180   .1280   .7724  2.
ATOM    CA    8    .1150   .2014   .2619  2.
ATOM    P     9    .0430   .4468   .2586  -1.
ATOM    P    10    .2075   .7726   .7768  -1.
ATOM    P    11    .2352   .0107   .2764  -1.
ATOM    P    12    .0564   .0714   .7584  -1.
ATOM    P    13    .4910   .8651   .2662  -1.
ATOM    P    14    .2992   .4745   .2495  -1.
@ EOF
   1   0   0
   0   0   1
   0   1   0
   0   0   1
@EOF
```

```
$$$$$$ THIS IS THE VERSION OF 1975 $$$$$$



@ADD,P M.TESTCK
       HA/OCP  MATCH LAYERS
 THE TOTAL THICKNESS OF THE SLICE IS TWICE   1.00 ANGSTROMS
 ATOMS MORE THAN      .75 ANGSTROMS FROM THE ATOM DEFINING THE CENTRAL PLANE
 WILL BE COUNTED UP AS FRINGE ATOMS TO ASCERTAIN THE ROUGHNESS OF THE PROPOSED SURFACE
 THE MOTIV RADIUS IS    6.00 ANGSTROMS
 A MAXIMUM OF    5 RECORDS WILL BE READ FROM UNIT  5, FILE  0.
     0 RECORDS WILL BE SKIPPED ON THE INPUT FILE BEFORE READ-IN BEGINS
 INPUT IN LATTICE VECTOR NOTATION, TWO VECTORS FOR EACH COMPOUND
 MATCHES WITH MERIT FIGURES ABOVE  4.00 WILL GENERATE LIST OF ATOMS ON SURFACE
 MAPS WILL ALSO BE DRAWN FOR THESE SLICES
 CONTENTS OF ATOM MOTIVS WILL BE WRITTEN OUT
 THE BEGINNING SLICES ARE   1 FOR COMPOUND A AND   1 FOR COMPOUND B
 ATOMS WITHIN 1.25 OF NEAREST DISTANCE FOR ATOMS OF THAT TYPE IN A MOTIV WILL BE INCLUDED IN MOTIV
 MOTIV VECTORS MUST MATCH WITHIN  .15*100 PERCENT
 CRYSTAL DATA FOR  1ST   COMPOUND
  REAL CELL IS  9.41510  9.41510  6.88100   .00000   .00000  -.50000
 RECIPROCAL CELL IS    .12264   .12264   .14533   .00000   .00000   .50000


 SYMMETRY ELEMENTS ARE
    T1 S11 S12 S13     T2 S21 S22 S23     T3 S31 S32 S33
  .000 -1.  0.  0.   .000  0. -1.  0.   .000  0.  0. -1.
  .000  1.  0.  0.   .000  0.  1.  0.   .000  0.  0.  1.
  .000 -1.  0.  0.   .000  0. -1.  0.   .500  0.  0.  1.
  .000  1.  0.  0.   .000  0.  1.  0.   .500  0.  0. -1.
  .000  0. -1.  0.   .000  1. -1.  0.   .000  0.  0.  1.
  .000  0.  1.  0.   .000 -1.  1.  0.   .500  0.  0.  1.
  .000  0.  1.  0.   .000 -1.  1.  0.   .000  0.  0. -1.
  .000  0. -1.  0.   .000  1. -1.  0.   .500  0.  0. -1.
  .000 -1.  1.  0.   .000 -1.  0.  0.   .000  0.  0.  1.
  .000  1. -1.  0.   .000  1.  0.  0.   .000  0.  0. -1.
  .000  1. -1.  0.   .000  1.  0.  0.   .500  0.  0.  1.
  .000 -1.  1.  0.   .000 -1.  0.  0.   .500  0.  0. -1.
 ATOM LIST IS
      ATOM       X         Y         Z     CHARGE
     CA    1  .33330   .66670   .00140 2.00
     CA    2  .24670   .99330   .25000 2.00
     P        .39850   .36840   .25000-1.00




 CRYSTAL DATA FOR  2ND   COMPOUND
  REAL CELL IS 19.66100  9.50900  6.82200  -.00297  -.04083  -.31582
 RECIPROCAL CELL IS    .05366   .11085   .14673   .01674   .04402   .31621


 SYMMETRY ELEMENTS ARE
    T1 S11 S12 S13     T2 S21 S22 S23     T3 S31 S32 S33
  .000  1.  0.  0.   .000  0.  1.  0.   .000  0.  0.  1.
  .000 -1.  0.  0.   .000  0. -1.  0.   .000  0.  0. -1.
 ATOM LIST IS
      ATOM       X         Y         Z     CHARGE
   1
```

```
CA    1   .07200   .79410   .00550 2.00
CA    2   .07060   .80580   .50370 2.00
CA    3   .36650   .03100   .02340 2.00
CA    4   .36310   .83530   .53390 2.00
CA    5   .10730   .44990   .76260 2.00
CA    6   .20120   .66010   .27570 2.00
CA    7   .21800   .12800   .77240 2.00
CA    8   .11500   .20140   .26190 2.00
P     9   .04300   .44680   .25860-1.00
P    10   .20750   .77260   .77680-1.00
P    11   .23520   .01070   .27640-1.00
P    12   .05640   .07140   .75840-1.00
P    13   .49100   .86510   .26620-1.00
P    14   .29920   .47450   .24950-1.00



16 UNIQUE ATOMS IN UNIT CELL
28 UNIQUE ATOMS IN UNIT CELL
```

```
EVALUATION OF A PROPOSED STRUCTURAL MATCH.
  DA1   DA2   DB1   DB2   ANGA   ANGB    VECTOR A1     VECTOR A2      VECTOR B1     VECTOR B2     DEL1   DEL2 DELANG RANK RECORD

  9.42  6.88  9.51  6.82  90.00  89.83 (   1   0   0,   0   0   1) (   0   1   0,   0   0   1)  .010  .009  .002  .115   1
AREA OF PLANE A IS    64.79AREA OF PLANE B IS    64.87 RATIO OF AREAS IS    .999
FRACTIONAL MISMATCH IS    .001  DISLOCATION DENSITY ASSUMMING NO ELASTIC STRAIN IS   .132+11
THE NEAREST INTEGER RATIO OF THE AREAS OF PLANE A AND PLANE B IS  1 TO   1
THESE YIELD A COMMON AREA OF   64.87 TAKEN AS THE AREA OF THE PATTERN REPEAT
THE NORMALS TO THE PLANES ARE    -.50   -1.00     .00 FOR COMPOUND A AND    1.00      .65      .12 FOR COMPOUND B
THESE NORMALS HAVE MULTIPLES OF THE REAL CELL TRANSLATIONS AS COMPONENTS

MILLER INDEX DESIGNATION OF PLANE DEFINED BY VECTOR NETWORK IS    .00  -1.00     .00 FOR COMPOUND A
AND     1.00       .00       .00 FOR COMPOUND B

SUBSEQUENT QUANTITIES ARE REFERRED TO AN ORTHOGONAL   COORDINATE SYSTEM,
X IS PARALLEL TO B CROSS C, Y IS PARALLEL TO C CROSS X, Z IS PARALLEL TO C.
DIRECTION COSINES AND D-SPACINGS FOR COMPOUNDS A AND B ARE
-.5000 -.8660  .0000   8.1537 AND 1.0000  .0000  .0000  18.6367 RESPECTIVELY



ATOMS REMAINING AFTER REDUNDANCIES AND SUBSETS REMOVED
COLUMNS ARE 1)SPACING FROM PLANE
            2)PLANE DEFINING ATOM
            3)ATOM IN SLICE WITH THIS SPACING
            4)ATOMIC COORDINATES IN ORTHOGONAL ANGSTROMS
            5)ASSIGNED ATOMIC CHARGE

     .00  CA   1  CA   1  5.4361  -.0005  6.8714 2.00
     .00  CA   1  CA   1  5.4361  -.0005  3.4501 2.00
     .65  CA   1  CA   2   .0546  2.3542  1.7202 2.00
     .71  CA   1  CA   2  2.0662  1.1298  5.1607 2.00
    -.29  CA   1  P       3.2493  1.5926  1.7202-1.00
    -.53  CA   1  P        .2454  3.6102  5.1607-1.00



ATOMS REMAINING AFTER REDUNDANCIES AND SUBSETS REMOVED
COLUMNS ARE 1)SPACING FROM PLANE
            2)PLANE DEFINING ATOM
            3)ATOM IN SLICE WITH THIS SPACING
            4)ATOMIC COORDINATES IN ORTHOGONAL ANGSTROMS
            5)ASSIGNED ATOMIC CHARGE

     .00  CA   1  CA   1  1.3418  7.1038  -.0427 2.00
    -.03  CA   1  CA   2  1.3157  7.2238  3.3568 2.00
     .66  CA   1  CA   5  1.9997  3.6116  5.1036 2.00
     .80  CA   1  CA   8  2.1432  1.2008  1.6887 2.00
    -.54  CA   1  P    9   .8014  3.9815  1.7170-1.00
    -.29  CA   1  P   12  1.0511   .3286  5.1265-1.00
     .00  CA   3  CA   3  6.8303 -1.9818  -.1355 2.00
    -.06  CA   3  CA   4  6.7670  5.6874  3.3272 2.00
     .00  CA   6  CA   6  3.7497  5.0271  1.7007 2.00
     .31  CA   6  CA   7  4.0628  -.1370  5.0907 2.00
     .12  CA   6  P   10  3.8671  6.0577  5.1109-1.00
     .63  CA   6  P   11  4.3833 -1.3593  1.6965-1.00
     .00  P   13  P   13  9.1506  5.1762  1.3974-1.00
     .34  P   13  P   13  9.4861 -1.8790  4.5935-1.00
```

```
COMPOUND A MOTIVS FOLLOW

MCTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
 CA    1  5.4361   -.0005   6.8714 2.00
 CA    1  5.4361   -.0005   3.4501 2.00
 CA    1  5.4361   -.0005  10.3311 2.00
 CA    2  2.0662   1.1298   5.1607 2.00
 CA    2  8.2083  -2.3533   8.6012 2.00
 P        3.2493   1.5926   8.6012-1.00
 P        8.3991  -1.0973   5.1607-1.00
MCTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
 CA    2   .0546   2.3542   1.7202 2.00
 CA    1 -2.7176   4.7071   -.0096 2.00
 CA    1 -2.7176   4.7071   3.4501 2.00
 CA    2  2.0662   1.1298  -1.7203 2.00
 CA    2  2.0662   1.1298   5.1607 2.00
 P        3.2493   1.5926   1.7202-1.00
          CA    2 IS A FRINGE ATOM IN SLICE BASED ON P
          CA    2 IS A FRINGE ATOM IN SLICE BASED ON P
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
 P        3.2493   1.5926   1.7202-1.00
 CA    1  5.4361   -.0005   -.0096 2.00
 CA    1  5.4361   -.0005   3.4501 2.00
 CA    2   .0546   2.3542   1.7202 2.00
 CA    2  2.0662   1.1298  -1.7203 2.00
 CA    2  2.0662   1.1298   5.1607 2.00
 P         .2454   3.6102  -1.7203-1.00
 P         .2454   3.6102   5.1607-1.00
         4 ATOMS IN FRINGE PART OF SLICE BASED ON ATOM  P
    4 ATOMS WERE IN FRINGE AREAS OF PLANES

CCMPOUND B MCTIVS FOLLOW

          CA    8 IS A FRINGE ATOM IN SLICE BASED ON CA    1
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
 CA    1  1.3418   7.1038   -.0427 2.00
 CA    2  1.3157   7.2238   3.3568 2.00
 CA    2  1.3157   7.2238  -3.4652 2.00
 CA    5  1.9997   3.6116  -1.7184 2.00
 CA    8  2.1432  10.7097   1.6604 2.00
 P     9   .8014   3.9815   1.7170-1.00
 P    12  1.0511   9.8376  -1.7237-1.00
         1 ATOMS IN FRINGE PART OF SLICE BASED ON ATOM  CA    1
          CA    8 IS A FRINGE ATOM IN SLICE BASED ON CA    2
MCTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
 CA    2  1.3157   7.2238   3.3568 2.00
 CA    1  1.3418   7.1038   -.0427 2.00
 CA    1  1.3418   7.1038   6.7793 2.00
 CA    5  1.9997   3.6116   5.1036 2.00
 CA    8  2.1432  10.7097   1.6604 2.00
 P     9   .8014   3.9815   1.7170-1.00
 P    12  1.0511   9.8376   5.0983-1.00
         1 ATOMS IN FRINGE PART OF SLICE BASED ON ATOM  CA    2
MCTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
 CA    5  1.9997   3.6116   5.1036 2.00
 CA    1  1.3418   7.1038   6.7793 2.00
 CA    2  1.3157   7.2238   3.3568 2.00
 CA    8  2.1432   1.2008   8.5107 2.00
```

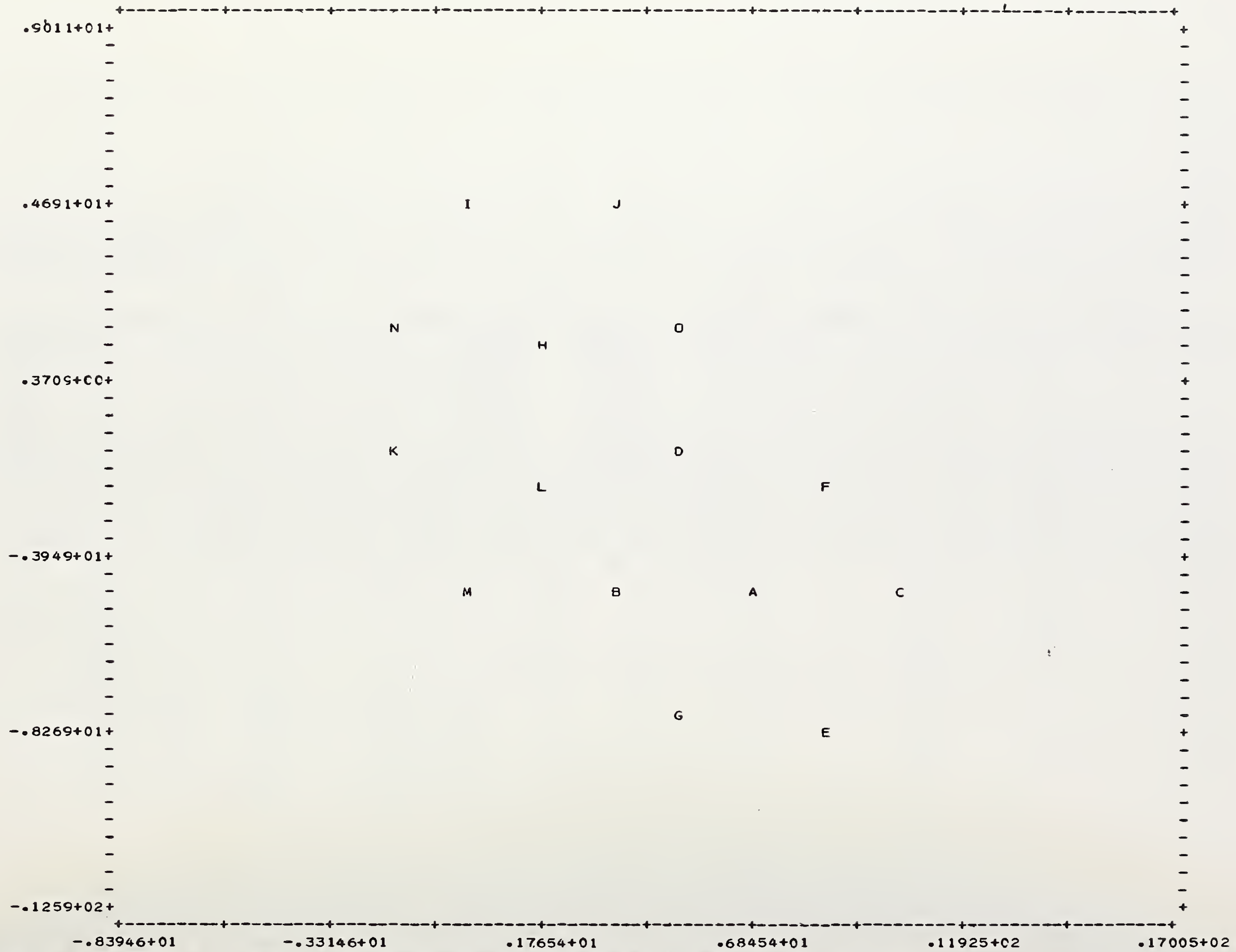
```
  CA    8  2.1432  1.2008  1.6887 2.00
  P    12  1.0511   .3286  5.1265-1.00
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
  CA    8  2.1432  1.2008  1.6887 2.00
  CA    1  1.3418 -2.4051  -.0145 2.00
  CA    2  1.3157 -2.2852  3.3850 2.00
  CA    5  1.9997  3.6116 -1.7184 2.00
  CA    5  1.9997  3.6116  5.1036 2.00
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
  P     9   .8014  3.9815  1.7170-1.00
  CA    1  1.3418  7.1038  -.0427 2.00
  CA    2  1.3157  7.2238  3.3568 2.00
  P    12  1.0511   .3286  5.1265-1.00
  P    12  1.0511   .3286 -1.6955-1.00
          CA    5 IS A FRINGE ATOM IN SLICE BASED ON P    12
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
  P    12  1.0511   .3286  5.1265-1.00
  CA    1  1.3418 -2.4051  6.8075 2.00
  CA    2  1.3157 -2.2852  3.3850 2.00
  CA    5  1.9997  3.6116  5.1036 2.00
  P     9   .8014  3.9815  1.7170-1.00
  P     9   .8014  3.9815  8.5390-1.00
         1 ATOMS IN FRINGE PART OF SLICE BASED ON ATOM  P    12
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
  CA    3  6.8303 -1.9818  -.1355 2.00
  CA    4  6.7670 -3.8216 -3.4666 2.00
  CA    4  6.7670 -3.8216  3.3554 2.00
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
  CA    4  6.7670  5.6874  3.3272 2.00
  CA    3  6.8303  7.5271  6.6583 2.00
  CA    3  6.8303  7.5271  -.1637 2.00
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
  CA    6  3.7497  5.0271  1.7007 2.00
  CA    7  4.0628  9.3719  5.0624 2.00
  CA    7  4.0628  9.3719 -1.7596 2.00
  P    10  3.8671  6.0577  5.1109-1.00
  P    10  3.8671  6.0577 -1.7111-1.00
  P    11  4.3833  8.1497  1.6682-1.00
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
  CA    7  4.0628  -.1370  5.0907 2.00
  CA    6  3.7497 -4.4819  1.7289 2.00
  CA    6  3.7497 -4.4819  8.5509 2.00
  P    10  3.8671 -3.4513  5.1392-1.00
  P    11  4.3833 -1.3593  1.6965-1.00
  P    11  4.3833 -1.3593  8.5185-1.00
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
  P    10  3.8671  6.0577  5.1109-1.00
  CA    6  3.7497  5.0271  1.7007 2.00
  CA    6  3.7497  5.0271  8.5227 2.00
  CA    7  4.0628  9.3719  5.0624 2.00
  P    11  4.3833  8.1497  8.4902-1.00
  P    11  4.3833  8.1497  1.6682-1.00
MOTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
  P    11  4.3833 -1.3593  1.6965-1.00
  CA    6  3.7497 -4.4819  1.7289 2.00
  CA    7  4.0628  -.1370  5.0907 2.00
  CA    7  4.0628  -.1370 -1.7313 2.00
  P    10  3.8671 -3.4513 -1.6828-1.00
```

```
 P    10   3.8671 -3.4513   5.1392-1.00
MCTIV(ATOM,COORDINATES IN ORTHOGONAL ANGSTROMS,CHARGE)
 P    13   9.1506   5.1762   1.3974-1.00
 P    13   9.4861   7.6299   4.5653-1.00
 P    13   9.4861   7.6299  -2.2567-1.00
    3 ATOMS WERE IN FRINGE AREAS OF PLANES


RESULTS FOR SLICE    1 VERSUS SLICE    1
               CA    1 CA    2 CA    5 CA    8 P     9 P    12
                     1       1       1       1       1       1
   CA    1    2  97.84   98.09   79.45   74.96   37.20   51.43
   CA    2    2  82.15   81.90   97.09   89.52   43.58   51.15
   P          2  59.79   59.40   51.17   52.05   70.92   86.03
SUM OF OCCURENCES OF ATOMS=    6 FOR A,    6 FOR B,MINIMUM=    6
MATCH  CA    1  CA    2    1    1       98.09       98.09     1     6
MATCH  CA    1  CA    1    2    1       97.84      195.93     2     6
MATCH  CA    2  CA    5    1    1       97.09      293.02     3     6
MATCH  CA    2  CA    8    2    1       89.52      382.54     4     6
MATCH  P        P    12    1    1       86.03      468.57     5     6
MATCH  P        P     9    2    1       70.92      539.49     6     6
SLICE    1 WITH SLICE    1, NETWORK MATCH NUMBER    0, SERIAL NUMBER    1 HAS FIT  8.3165

PLOT FOR PLANE A


PLOT AXIS AND ROTATION ANGLES FOR PLOT ARE    -.00000     .00000    8.15372 -60.00000 -90.00000
```

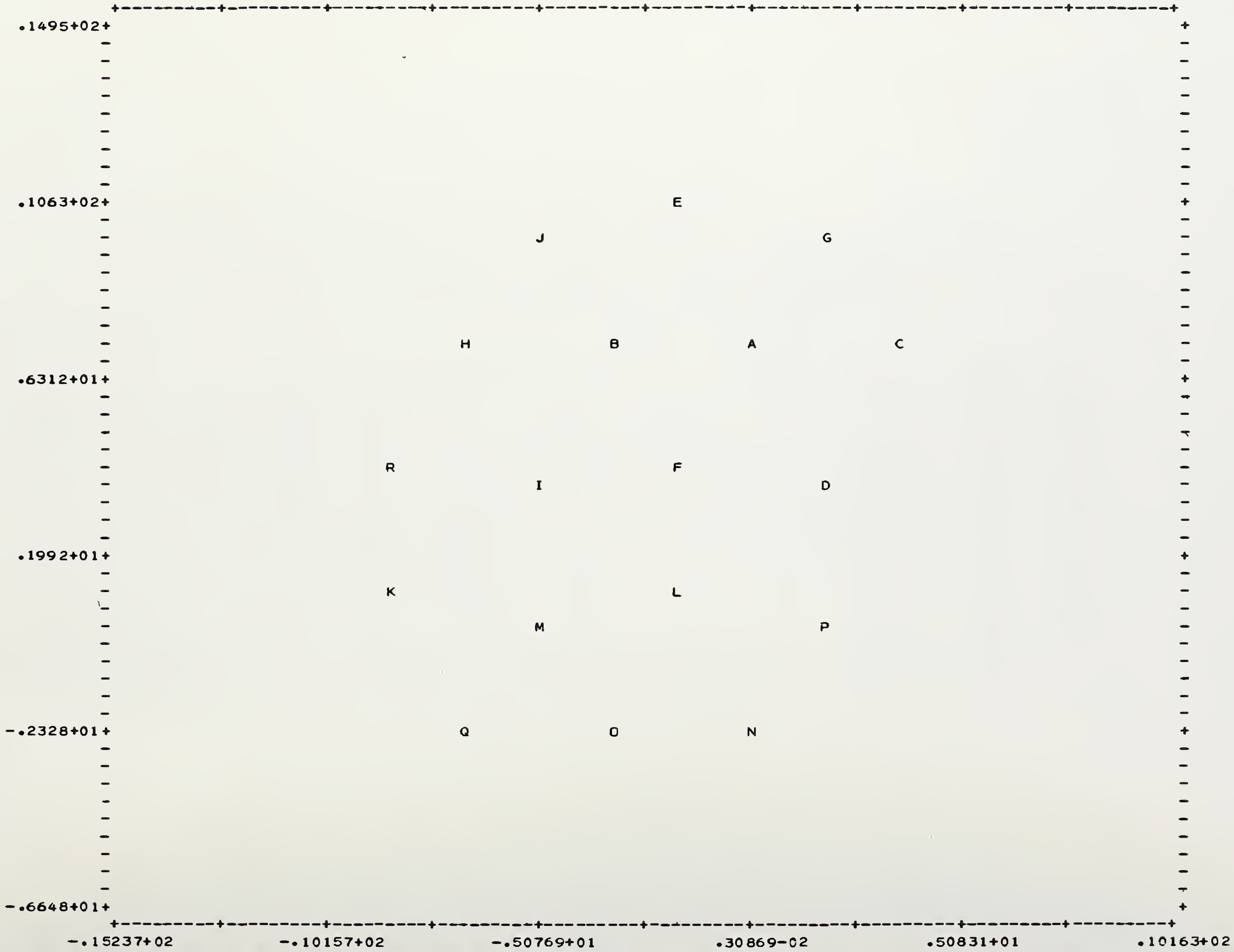


PLOT HAS A CONSTANT SCALE OF 1 CM = 1 ANGSTROM OR 10* *8 MAGNIFICATION.
CENTER OF PLOT IS (4.305, -1.789). XMIN= -1.720 XMAX= 10.331 YMIN= -8.285 YMAX= 4.707

```
ATOMS AS PROJECTED ONTO SURFACE(SYMBOL,ORTHOGONAL COORDINATES,CHARGE. FRACTIONAL CRYSTAL COORDINATES. X,Y,Z
CRYSTAL COORDINATES AID IN DETERMINIMG THE TRANSLATIONAL SYMMETRY ON THE MAP SHOWN ABOVE
      1    A    CA   1  6.8714 -4.7080 -2.7176   2.00                                 .6667   .3333   .9986
      2    B    CA   1  3.4501 -4.7080 -2.7176   2.00                                 .6667   .3333   .5014
      3    C    CA   1 10.3311 -4.7080 -2.7176   2.00                                 .6667   .3333  1.5014
      4    D    CA   2  5.1607 -1.2244 -2.0115   2.00                                 .2534   .2467   .7500
      5    E    CA   2  8.6012 -8.2853 -2.0662   2.00                                1.0067   .2534  1.2500
      6    F    P       8.6012 -2.0177 -3.0038  -1.00                                 .3965   .3684  1.2500
      7    G    P       5.1607 -7.8225 -3.2493  -1.00                                1.0301   .3985   .7500
      8    H    CA   2  1.7202  1.1298 -2.0662   2.00                                 .0067   .2534   .2500
      9    I    CA   1  -.0096  4.7071 -2.7176   2.00                                -.3333   .3333  -.0014
     10    J    CA   1  3.4501  4.7071 -2.7176   2.00                                -.3333   .3333   .5014
     11    K    CA   2 -1.7203 -1.2244 -2.0115   2.00                                 .2534   .2467  -.2500
     12    L    P       1.7202 -2.0177 -3.0038  -1.00                                 .3985   .3684   .2500
     13    M    CA   1  -.0096 -4.7080 -2.7176   2.00                                 .6667   .3333  -.0014
     14    N    P      -1.7203  1.5926 -3.2493  -1.00                                 .0301   .3965  -.2500
     15    O    P       5.1607  1.5926 -3.2493  -1.00                                 .0301   .3985   .7500

PLOT FOR PLANE B


PLOT AXIS AND ROTATION ANGLES FOR PLOT ARE     .00000     .00000  18.63665     .00000  90.00000
```



PLOT HAS A CONSTANT SCALE OF 1 CM = 1 ANGSTROM OR 10* *8 MAGNIFICATION.
CENTER OF PLOT IS (-2.537,   4.152), XMIN=   -8.539 XMAX=   3.465 YMIN=   -2.405 YMAX=   10.710

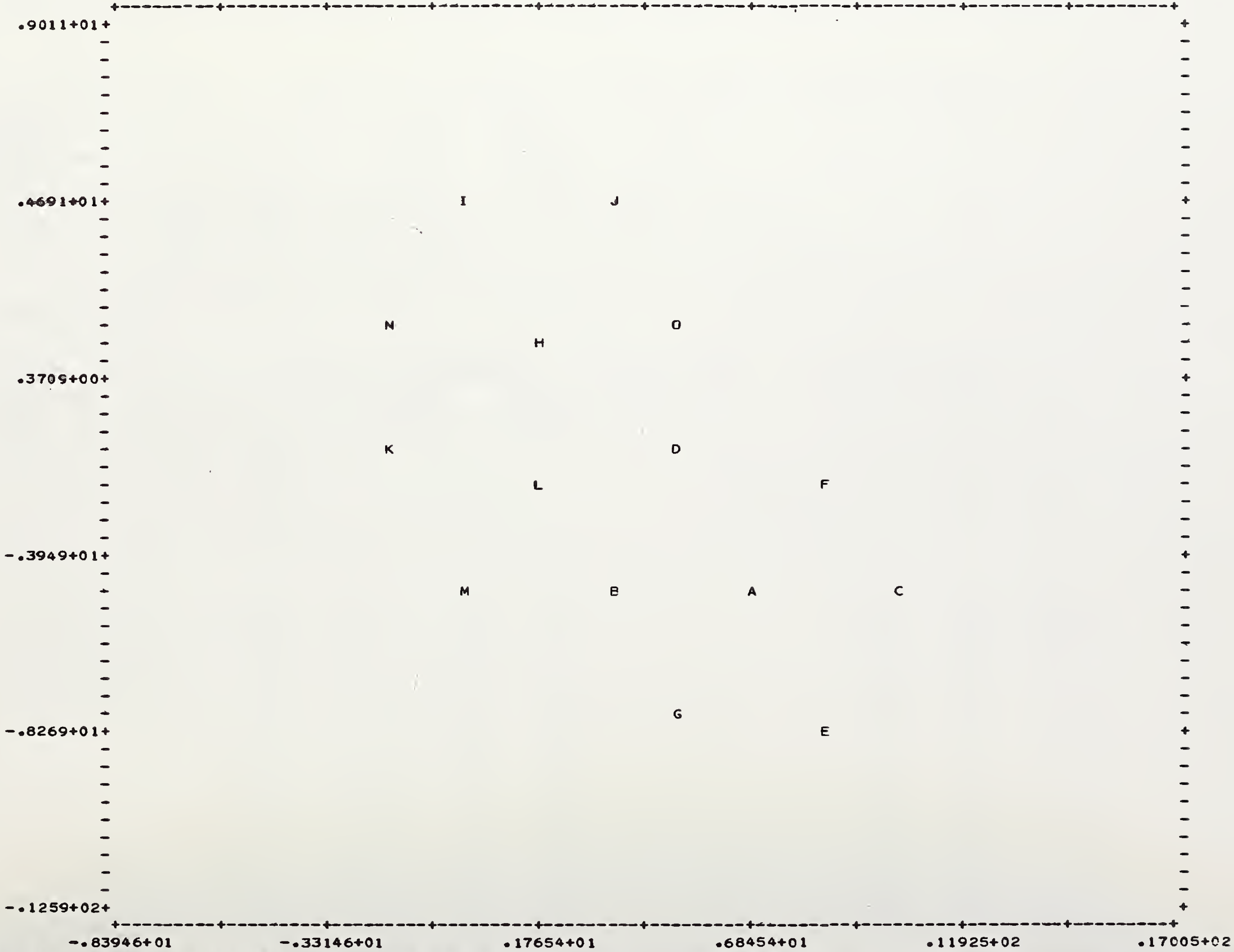
```
ATOMS AS PROJECTED ONTO SURFACE(SYMBOL,ORTHOGONAL COORDINATES,CHARGE. FRACTIONAL CRYSTAL COORDINATES, X,Y,Z
CRYSTAL COORDINATES AID IN DETERMINIMG THE TRANSLATIONAL SYMMETRY ON THE MAP SHOWN ABOVE
     1   A   CA   1    .0427   7.1038   1.3418    2.00                           .0720    .7941    .0055
     2   B   CA   2  -3.3568   7.2238   1.3157    2.00                           .0706    .8058    .5037
     3   C   CA   2   3.4652   7.2238   1.3157    2.00                           .0706    .8058   -.4963
     4   D   CA   5   1.7184   3.6116   1.9997    2.00                           .1073    .4499   -.2374
     5   E   CA   8  -1.6604  10.7097   2.1432    2.00                           .1150   1.2014    .2619
     6   F   P    9  -1.7170   3.9815    .8014   -1.00                           .0430    .4468    .2586
     7   G   P   12   1.7237   9.8376   1.0511   -1.00                           .0564   1.0714   -.2416
     8   H   CA   1  -6.7793   7.1038   1.3418    2.00                           .0720    .7941   1.0055
     9   I   CA   5  -5.1036   3.6116   1.9997    2.00                           .1073    .4499    .7626
    10   J   P   12  -5.0983   9.8376   1.0511   -1.00                           .0564   1.0714    .7584
    11   K   CA   8  -8.5107   1.2008   2.1432    2.00                           .1150    .2014   1.2619
    12   L   CA   8  -1.6887   1.2008   2.1432    2.00                           .1150    .2014    .2619
    13   M   P   12  -5.1265    .3286   1.0511   -1.00                           .0564    .0714    .7584
    14   N   CA   1    .0145  -2.4051   1.3418    2.00                           .0720   -.2059    .0055
    15   O   CA   2  -3.3850  -2.2852   1.3157    2.00                           .0706   -.1942    .5037
    16   P   P   12   1.6955    .3286   1.0511   -1.00                           .0564    .0714   -.2416
    17   Q   CA   1  -6.8075  -2.4051   1.3418    2.00                           .0720   -.2059   1.0055
    18   R   P    9  -8.5390   3.9815    .8014   -1.00                           .0430    .4468   1.2586


RESULTS FOR SLICE    1 VERSUS SLICE    1
                CA    3 CA    4
                      1       1
    CA    1    2  58.03  58.03
    CA    2    2  65.85  65.85
    P          2  40.71  40.71
SUM OF OCCURENCES OF ATOMS=    6 FOR A,    2 FOR B,MINIMUM=    2
MATCH  CA    2  CA    4    1    1      65.85      65.85     1     2
MATCH  CA    2  CA    3    2    1      65.85     131.70     2     2
SLICE    1 WITH SLICE    1, NETWORK MATCH NUMBER    0, SERIAL NUMBER    2 HAS FIT  2.0302


RESULTS FOR SLICE    1 VERSUS SLICE    1
                CA    6 CA    7 P    10 P    11
                      1       1       1       1
    CA    1    2  70.87  71.58  51.58  50.87
    CA    2    2  58.81  59.35  39.35  38.81
    P          2  51.18  51.60  71.60  71.18
SUM OF OCCURENCES OF ATOMS=    6 FOR A,    4 FOR B,MINIMUM=    4
MATCH  P         P   10    1    1      71.60      71.60     1     4
MATCH  CA    1  CA    7    1    1      71.58     143.18     2     4
MATCH  P         P   11    2    1      71.18     214.36     3     4
MATCH  CA    1  CA    6    2    1      70.87     285.23     4     4
SLICE    1 WITH SLICE    1, NETWORK MATCH NUMBER    0, SERIAL NUMBER    3 HAS FIT  4.3969

PLCT FOR PLANE A


PLOT AXIS AND ROTATION ANGLES FOR PLOT ARE    -.00000     .00000    8.15372 -60.00000 -90.00000
```



```
PLOT HAS A CONSTANT SCALE OF 1 CM = 1 ANGSTROM OR 10* *8 MAGNIFICATION.
CENTER OF PLOT IS (    4.305,  -1.789), XMIN=    -1.720 XMAX=    10.331 YMIN=    -8.285 YMAX=     4.707
```

```
ATCMS AS PROJECTED ONTO SURFACE(SYMBOL.ORTHOGONAL COORDINATES.CHARGE. FRACTIONAL CRYSTAL COORDINATES, X,Y,Z
CRYSTAL COORDINATES AID IN DETERMINIMG THE TRANSLATIONAL SYMMETRY ON THE MAP SHOWN ABOVE
     1   A   CA   1  6.8714 -4.7080 -2.7176   2.00                          .6667   .3333   .9986
     2   B   CA   1  3.4501 -4.7080 -2.7176   2.00                          .6667   .3333   .5014
     3   C   CA   1 10.3311 -4.7080 -2.7176   2.00                          .6667   .3333  1.5014
     4   D   CA   2  5.1607 -1.2244 -2.0115   2.00                          .2534   .2467   .7500
     5   E   CA   2  8.6012 -8.2853 -2.0662   2.00                         1.0067   .2534  1.2500
     6   F   P       8.6012 -2.0177 -3.0038  -1.00                          .3985   .3684  1.2500
     7   G   P       5.1607 -7.8225 -3.2493  -1.00                         1.0301   .3985   .7500
     8   H   CA   2  1.7202  1.1298 -2.0662   2.00                          .0067   .2534   .2500
     9   I   CA   1  -.0096  4.7071 -2.7176   2.00                         -.3333   .3333  -.0014
    10   J   CA   1  3.4501  4.7071 -2.7176   2.00                         -.3333   .3333   .5014
    11   K   CA   2 -1.7203 -1.2244 -2.0115   2.00                          .2534   .2467  -.2500
    12   L   P       1.7202 -2.0177 -3.0038  -1.00                          .3985   .3684   .2500
    13   M   CA   1  -.0096 -4.7080 -2.7176   2.00                          .6667   .3333  -.0014
    14   N   P      -1.7203  1.5926 -3.2493  -1.00                          .0301   .3985  -.2500
    15   O   P       5.1607  1.5926 -3.2493  -1.00                          .0301   .3985   .7500

PLOT FOR PLANE B


PLOT AXIS AND ROTATION ANGLES FOR PLOT ARE     .00000     .00000  18.63665    .00000  90.00000
```

```
PLOT HAS A CONSTANT SCALE OF 1 CM = 1 ANGSTROM OR 10* *8 MAGNIFICATION.
CENTER OF PLOT IS (  -3.396,    2.445), XMIN=   -8.551 XMAX=    1.760 YMIN=   -4.482 YMAX=    9.372
```

```
ATOMS AS PROJECTED ONTO SURFACE(SYMBOL,ORTHOGONAL COORDINATES,CHARGE. FRACTIONAL CRYSTAL COORDINATES, X,Y,Z
CRYSTAL CCORDINATES AID IN DETERMINIMG THE TRANSLATIONAL SYMMETRY ON THE MAP SHOWN ABOVE
     1    A    CA    6 -1.7007   5.0271   3.7497    2.00                                     .2012    .6601    .2757
     2    B    CA    7 -5.0624   9.3719   4.0628    2.00                                     .2180   1.1280    .7724
     3    C    CA    7  1.7596   9.3719   4.0628    2.00                                     .2180   1.1280   -.2276
     4    D    P    10 -5.1109   6.0577   3.8671   -1.00                                     .2075    .7726    .7768
     5    E    P    10  1.7111   6.0577   3.8671   -1.00                                     .2075    .7726   -.2232
     6    F    P    11 -1.6682   8.1497   4.3833   -1.00                                     .2352   1.0107    .2764
     7    G    CA    7 -5.0907   -.1370   4.0628    2.00                                     .2180    .1280    .7724
     8    H    CA    6 -1.7289  -4.4819   3.7497    2.00                                     .2012   -.3399    .2757
     9    I    CA    6 -8.5509  -4.4819   3.7497    2.00                                     .2012   -.3399   1.2757
    10    J    P    10 -5.1392  -3.4513   3.8671   -1.00                                     .2075   -.2274    .7768
    11    K    P    11 -1.6965  -1.3593   4.3833   -1.00                                     .2352    .0107    .2764
    12    L    P    11 -8.5185  -1.3593   4.3833   -1.00                                     .2352    .0107   1.2764
    13    M    CA    6 -8.5227   5.0271   3.7497    2.00                                     .2012    .6601   1.2757
    14    N    P    11 -8.4902   8.1497   4.3833   -1.00                                     .2352   1.0107   1.2764
    15    O    CA    7  1.7313   -.1370   4.0628    2.00                                     .2180    .1280   -.2276
    16    P    P    10  1.6828  -3.4513   3.8671   -1.00                                     .2075   -.2274   -.2232

RESULTS FOR SLICE   1 VERSUS SLICE   1
               P   13
                    2
   CA   1   2  36.96
   CA   2   2    .00
   P        2  51.99
SUM OF OCCURENCES OF ATOMS=   6 FOR A.   2 FOR B.MINIMUM=   2
MATCH  P        P   13   1   1      51.99     51.99    1    2
MATCH  P        P   13   2   2      51.99    103.99    2    2
SLICE   1 WITH SLICE   1, NETWORK MATCH NUMBER   0, SERIAL NUMBER   4 HAS FIT  1.6030
```

```
  4 BEST MATCHES BETWEEN COMPOUNDS A AND B
VALUES SCALED TO UNIT AREA FOR EACH MATCH PLANE
TCTAL NUMBER OF MATCHES  FCR COMPOUNDS IS   4
  SLICE A   SLICE B   NETWORK       FIT
                         PAIR
        1         1         0      8.32
        1         1         0      4.40
        1         1         0      2.03
        1         1         0      1.60
JCB COMPLETED
```

NBS-114A (REV. 7-73)

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5. Publication Date

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7. AUTHOR(S)

Brian Dickens and LeRoy W. Schroeder*

8. Performing Organ. Report No.

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* American Dental Association
Health Foundation Research Unit
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13. Type of Report & Period Covered

14. Sponsoring Agency Code

15. SUPPLEMENTARY NOTES

16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

Two computer programs to evaluate possible structural matches for use in epitaxy and twinning studies have been written in FORTRAN V for the UNIVAC 1108. They should be readily convertible to other comparable computers.

The first program, MATCH1, requires knowledge of the unit cell parameters. It obtains all matching networks in two unit cell lattices and sorts the matches into an order of probable epitaxy (or twinning if the two unit cells are the same) based solely on criteria of dimensional mismatch and network area.

The second program, MATCH2, requires knowledge of positional parameters of the atoms in the crystal structures. It calculates the degree of structural fit for slices supplied from visual inspection of the crystal structures or as matching networks determined by MATCH1.

The slice comparison is carried out in terms of the vector set of the environment of each atom in each slice. The procedure is not valid when the twin operation is a rotation about the normal of the compositional plane or a reflection in a mirror parallel to this plane. The atomic patterns comprising the slices are matched piece by piece in MATCH2. A third program, MATCH3, will match whole patterns once three fiducial atoms in each pattern have been picked from the output of MATCH2 and will handle all the twinning cases. MATCH3 will be described in a future National Bureau of Standards Technical Note.

Cont.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)*

computer calculations; crystal structure; epitaxy; lattice misfit; pattern recognition; twinning

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19. SECURITY CLASS (THIS REPORT) UNCLASSIFIED	21. NO. OF PAGES 71
20. SECURITY CLASS (THIS PAGE) UNCLASSIFIED	22. Price $1.30

ABSTRACT--continued

This Technical Note explains the procedure in MATCH1 and MATCH2 and includes listings of the programs and examples of results. The programs are available on magnetic tape or card decks obtainable from the authors.

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