

## The Crystallography of the Austenite-Martensite Transformation in an Fe-Cr-C Alloy

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An analysis of the crystallography of the austenite-martensite transformation in a high purity Fe-Cr-C alloy was made. Lattice parameters of the two phases, the austenite-martensite orientation relationship, and the habit plane of the martensite were determined experimentally. Considerably less scatter in habit plane poles was observed than has been reported by others for a similar alloy. None of the existing crystallographic theories adequately explains the results, and it is suggested that an additional anisotropic interface distortion be incorporated into the theory. An inverse method of analysis for determining the pattern of inhomogeneity is discussed, with particular reference to the orientation relationship, and it is shown that the orientation relationship is a comparatively inaccurate quantity when used in theoretical calculations.

### Introduction

Based on the principle of an undistorted and unrotated habit plane, recent crystallographic analyses of diffusionless phase transformations have led to the consideration of the total transformation distortion (shape deformation) as a pure lattice deformation (Bain strain) coupled with a lattice invariant deformation (inhomogeneous shear) such as fine scale slip or twinning, and a rigid body rotation. The theory of Wechsler-Lieberman-Read (WLR) (1953) (which is equivalent to the later analyses of Bilby & Bullough (1956), and Bilby & Frank (1960)) is based on an interface plane which is undistorted and unrotated. The theory of Bowles-Mackenzie (1954*a, b, c*) (BM) treats the interface plane as one which is unrotated, but possibly (uniformly) dilated. In the case of iron alloys, WLR (1960) proposed to account for a variation in habit plane and orientation relationship, *etc.*, by a variation in the lattice invariant shear system, maintaining the requirement that the interface remains macroscopically undistorted, while BM adhered to one particular shear system, but permitted the interface dilation to vary, thus causing a change in the habit plane and other crystallographic features with a dilation parameter. In this paper, the approaches of BM and WLR have been used to analyze the crystallographic aspects of the martensite transformation in an alloy consisting of Fe-1.51 wt.% C-3.09 wt.% Cr. For this alloy, an experimental determination of the lattice parameters of the austenite and martensite, the habit plane of the martensite, and the lattice orientation relationship between the two phases was made.

### Theoretical

According to the theory of WLR the shape deformation is given by the matrix  $E$ , which will not in general generate the product lattice from the parent lattice. This matrix describes the displacement of surface scratches inscribed on a specimen prior to its transformation from the parent into the product. The decomposition of the matrix  $E$  by WLR was done in the following way:

$$E = RPG \quad (1)$$

where  $R$  is a rotation matrix,  $P$  is the lattice deformation (Bain strain), and  $G$  is a lattice invariant shear of amount  $g$  on a certain plane and in a certain direction. All matrices in (1) are given with respect to an orthogonal set of axes along the austenite cube edges. Equation (1) can also be written as

$$E = RG_m P \quad (2)$$

where the lattice invariant shear,  $G_m$ , occurs in the martensite lattice. However, it is more convenient (mathematically) to consider the lattice invariant shear to occur in the austenite. The matrix  $G$  represents an invariant plane strain because it is a simple shear.  $E$  is also an invariant plane strain since this matrix represents a simple shear on the habit plane coupled with a normal component due to the volume change of the transformation. The matrices  $E^{-1}$  and  $G^{-1}$  also represent invariant plane strains since the inverse of an invariant plane strain is itself an invariant plane strain (Bowles & Mackenzie, 1954*a*).

The analysis of BM is exactly equivalent to that

of WLR when the interface plane is undilated. Essentially, BM wrote equation (1) in the form (for no interface dilation).

$$EG^{-1} = RP \quad (3)$$

where, as was pointed out,  $RP$  is an invariant line strain. The resultant of two invariant plane strains (due to  $E$  and  $G^{-1}$ ) is an invariant line strain, along the line of intersection of the two planes (the habit plane and the shear plane) which are invariant.

In the case where the interface plane is assumed to be uniformly dilated (*i.e.*, the  $\{225\}_A$  transformation in steels) the shape deformation is given by the matrix  $E/\delta$  where  $\delta$  is a scalar having values between 1.00 and 1.02 for steels. That is,  $E/\delta$  is an invariant plane strain. The corresponding invariant line strain is then  $L = \delta RP$ , *i.e.*, the near unity eigenvalue corresponding to the unrotated line of the matrix  $RP$  differs from unity by a factor  $\delta$ .

The elements of the matrix  $P$  are known from the lattice parameters of the two phases and the (assumed) lattice correspondence. The rotation matrix  $R$  can always be determined if the lattice orientation relationship is known, because  $R$  is the rotation which takes vectors and normals in the as-Bain-strained position to their final position in the martensite. Or, alternatively,  $R$  may be viewed in the following way (Bullough & Bilby, 1956). The application of  $PG$  to any vector in the habit plane causes this vector to undergo a rotation exactly opposite to that produced by the application of  $R$  to the same vector. That is,  $R$  ensures that the habit plane is unrotated.

In the case of known transformations in iron alloys, the matrix  $RP$  has three real eigenvalues; one of these three eigenvalues is within a percent or two of unity. The eigenvector corresponding to the near-unity eigenvalue represents the unrotated and potentially invariant line. In the absence of an interface dilation (WLR) the eigenvalue is exactly unity, but in the case of the BM theory, differs from unity by a small dilation.

Historically, the martensite problem has been treated by using as input data the known lattice parameters (and correspondence) and an assumed plane and direction for the lattice invariant shear. The solution to the problem gives the amount of lattice invariant shear,  $g$ , the habit plane left invariant by  $E$ , and the elements of the matrices  $E$  and  $R$ .

Theoretically, if certain information is known from experiment, the inverse problem can be worked to recover the system of the lattice invariant shear. This problem is particularly intriguing because of recent experimental determinations of the fine structure in martensitic phases by transmission electron microscopy. If the lattice parameters, orientation relationship, and habit plane are known, one can in

principle determine the plane, direction, and amount of lattice invariant shear (hence the matrix  $G$ ), and the matrix  $E$  (hence the shape deformation). The inverse problem was described graphically by Lieberman (1958) for iron alloys, and BM (1954*b*) indicated how some information can be recovered analytically. Graphical analysis lacks the precision attainable by the matrix method, and in some degenerate cases the graphical method cannot be used.

An inverse analytical method for recovering the elements of  $G$  is briefly described. The matrix  $R$  can be obtained by applying Euler's theorem for solid body rotations. If the positions of two non-collinear vectors (or plane normals) are known (from the orientation relationship) and if the positions of these same vectors (or normals) due to the strain  $\delta P$  (or  $(\delta P)^{-1}$ ) are known (this is always known from the lattice parameters and correspondence), an axis of rotation and an amount of rotation to make the Bain-strained positions of the vectors (normals) coincide with the final positions can be determined. If  $\mathbf{u}_i$  is unit rotation axis and the amount of rotation is  $\theta$ , then the generalized rotation matrix  $R$  (with respect to the austenite axis system) is given by

$$R_{ij} = \delta_{ij} \cos \theta + u_i u_j (1 - \cos \theta) - \varepsilon_{ijk} u_k \sin \theta \quad (4)$$

where  $\delta_{ij}$  is the Kronecker delta and  $\varepsilon_{ijk}$  is a permutation symbol.

Since  $R$  and  $P$  are known from experimental determinations of the orientation relationship and lattice parameters, the appropriate eigenvector (invariant line) can be found from the equation

$$(RP - \lambda I)\mathbf{X}_i = 0 \quad (5)$$

where  $I$  is the identity matrix and  $\mathbf{X}_i$  is the unrotated line. The dilation can be obtained from the condition

$$\delta\lambda = 1. \quad (6)$$

The habit plane normal is known from experiment, and arbitrary vectors  $\mathbf{v}$  in the habit plane are given by

$$\mathbf{v} = \mathbf{k} \times \mathbf{n} \quad (7)$$

where  $\mathbf{k}$  is any unit vector, and  $\mathbf{n}$  is a unit vector along the habit plane normal. It has been shown (Bowles & Mackenzie, 1954*a*) that the displacement of an arbitrary vector in the habit plane by the invariant line strain is in the same direction as the vector  $L\mathbf{d}_2$ , where  $\mathbf{d}_2$  is the direction of the lattice invariant shear. That is,

$$(L - I)\mathbf{v} \parallel L\mathbf{d}_2. \quad (8)$$

Thus the direction of the lattice invariant shear is given by

$$\mathbf{d}_2 \parallel L^{-1}(L - I)\mathbf{v}. \quad (9)$$

Since both the invariant line,  $\mathbf{l}$ , and shear direction,

$\mathbf{d}_2$ , must lie in the shear plane,  $\mathbf{p}_2$ , it follows that the shear plane normal,  $\mathbf{p}_2$ , is given by\*

$$\mathbf{p}_2 = \mathbf{l} \times \mathbf{d}_2 . \quad (10)$$

### Experimental procedure

The alloy studied was triply vacuum melted, prepared from high purity materials, and was analyzed to contain Fe-3.09 wt.% Cr-1.51 wt.% C. To ensure complete carbide dissolution and homogeneous austenite, the alloy was austenitized 100 hours at 1228 °C. Austenitizing was done in evacuated quartz capsules, and the resulting austenite grain size was from 2 to 6 mm. No change in composition of the specimens during heat treatment could be detected by chemical analysis. All specimens were quenched from 1228 °C to room temperature, and were entirely austenitic at room temperature. The  $M_s$  temperature was found to be between -14 and -18 °C after further cooling, and it was observed that this alloy exhibited the 'burst' phenomenon.

The detailed procedure for determining habit planes, orientation relationships, and lattice parameters has already been described in connection with another investigation (Wayman *et al.*, 1961). All Laue photographs were taken with a microbeam X-ray unit, and lattice parameters were determined by means of a diffractometer. One orientation photograph exhibiting both martensite and austenite Laue spots was obtained by polishing parallel to a particular martensite plate whose habit plane direction cosines were previously determined.

Four different specimens were studied, and twelve habit plane determinations were made. All habit plane determinations were made on relatively long martensite plates, where the plane of the plate and the plane of the midrib were not significantly different. The large plates presumably resulted from the lengthy heat treatment and large austenite grain size. However, it was observed that when some smaller plates formed, there was as much as seven degrees difference between the plane of the midrib and the mean plane of the plate. In addition, the midribs of the smaller plates ( $hkl$ ) which formed near larger plates ( $hkl$ ) were parallel to the larger plates, although the smaller plates themselves were not necessarily exactly parallel to the larger plates. In other words, midribs appeared parallel although plates were not necessarily parallel.

### Experimental results

The results of the habit plane determinations for the subject alloy are given in Table 1. These results are plotted on a common unit triangle in Fig. 1. It can be seen that all habit plane poles fell within a two

\* The  $\{225\}_A$  case is degenerate since the invariant line and shear direction are the same,  $\langle 011 \rangle_A$ .

Table 1. Results of habit plane determinations, Fe-1.51C-3.09Cr

Specimen no.	Plate	Direction cosines*
27	<i>a, b, c, d</i>	0.899
		0.364
		0.244
	<i>e, f, g</i>	0.890
		0.382
		0.250
29	<i>a</i>	0.887
		0.375
		0.268
30	<i>a</i>	0.887
		0.380
		0.259
	<i>b</i>	0.890
		0.391
		0.254
33	<i>a</i>	0.900
		0.367
		0.234
	<i>b</i>	0.886
		0.367
		0.282

\* Permuted to common variant.

and one-half degree solid angle. Furthermore, the habit plane was neither  $\{225\}_A$  nor  $\{259\}_A$  as is usually found for high carbon steels. This makes it clear that for iron alloys, habit planes between  $\{225\}$  and  $\{259\}$  do exist. A similar result was obtained by Otte & Read (1957), who examined an alloy of nominal composition Fe-1.5C-2.8Cr, but in this case,

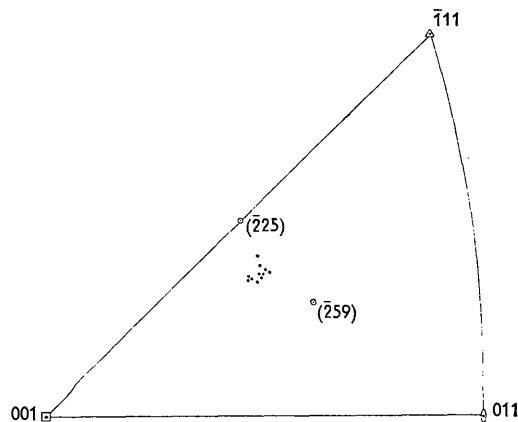


Fig. 1. Results of twelve habit plane determinations for Fe-1.51C-3.09Cr. All poles have been permuted to a common habit plane variant with respect to austenite. See Table 1 for Miller indices.

an extraordinary scatter in habit plane poles was observed. The scatter is probably in part due to the smallness of the plates investigated (shown at 1400× in Otte & Read (1957) as compared with 100× in the present work). With such small plates, a good

deal of arbitrariness is involved in making a decision as to what the habit plane may in fact be. Moreover, the alloy studied was not chemically analyzed after treatment, and the lattice parameters and orientation relationship were not determined.

The orientation relationship was determined from the stereographic projection to be

$$\begin{array}{lll} (111)_A & 0.3^\circ & \text{from } (011)_M \\ [01\bar{1}]_A & 2.8^\circ & \text{from } [11\bar{1}]_M \\ [\bar{1}10]_A & 6.1^\circ & \text{from } [\bar{1}\bar{1}\bar{1}]_M. \end{array}$$

Because of the smeared nature of the Laue spots from the martensite, the  $(011)_M$  and  $(111)_A$  reflections nearly overlapped. However, a distinction between the two reflections could be made, and their separation appeared to be  $0.3^\circ$ . In addition, when an orientation relationship is determined by polishing parallel to a martensite plate, the plane of the stereographic projection becomes essentially the habit plane. Within the limits of observation,  $(111)_A$ ,  $(011)_M$ , and the habit plane were cozoal, with the  $(011)_M$  reflection lying between  $(111)_A$  and the habit plane. This orientation relationship is plotted stereographically in Fig. 2.

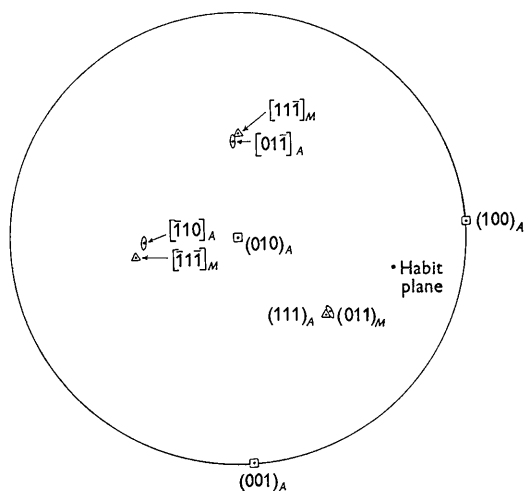


Fig. 2. Stereographic projection showing orientation relationship between martensite and austenite. The orientation relationship was obtained by polishing parallel to a martensite plane whose direction cosines were previously determined to be  $(0.890, 0.382, 0.250)$  with respect to the austenite.

These results can be compared to the Greninger-Troiano orientation relationship:

$$\begin{array}{lll} (111)_A & || & (011)_M \quad \text{within } 1^\circ \\ [01\bar{1}]_A & & 2.5^\circ \quad \text{from } [11\bar{1}]_M \\ [\bar{1}10]_A & & 6.5^\circ \quad \text{from } [\bar{1}\bar{1}\bar{1}]_M. \end{array}$$

The lattice parameters were found to be

$$\begin{array}{l} \text{Austenite: } a_0 = 3.626 \text{ \AA} . \\ \text{Martensite: } a = 2.854 \text{ \AA}, c = 3.060 \text{ \AA}; c/a = 1.0722 . \end{array}$$

## Discussion

It is interesting to consider the theoretical predictions of the crystallographic features of the transformation for this alloy. Because of recent observations (Nutting & Kelly, 1960; Nishiyama, 1960) of  $\{112\}_M$  twinning in several iron alloys which exhibit both the  $\{225\}_A$  and  $\{259\}_A$  type habits, it is the most reasonable assumption to consider that the transformation inhomogeneity or lattice invariant shear is of the  $\{112\}_M \langle 111 \rangle_M$  type. The analysis of this alloy has been based on the assumption of  $\{112\}_M$  inhomogeneity (equivalently  $\{011\}_A$ ).

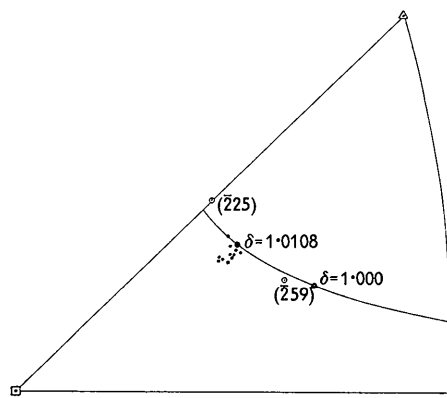


Fig. 3. Experimentally determined habit planes and the theoretical variation of the habit plane with the parameter delta according to the theory of Bowles & Mackenzie. The best agreement between theory and experiment was obtained with  $\delta = 1.0108$ .

WLR derived an expression for the habit plane direction cosines in terms of the elements of the Bain strain matrix by assuming that the lattice invariant shear system was  $\{112\}_M \langle 111 \rangle_M$ . These expressions are given in Wechsler *et al.* (1953) as equations (32), (33), and (34). If one substitutes  $\delta\eta_i$  for  $\eta_i$  in these expressions, the habit plane for a given uniform dilation,  $\delta$ , can be determined (Christian, 1955). Fig. 3 shows the variation of the predicted habit plane with the dilation parameter,  $\delta$ , as well as the experimental habit plane determinations. As has been shown (Wechsler *et al.*, 1953) the WLR analysis ( $\delta=1$ ) predicts essentially the  $\{259\}_A$  type habit plane, in considerable disagreement with the observed habit plane for this alloy. In fact, WLR examined a wide range of volume ratios and axial ratios with the assumption of  $\{112\}_M$  twinning, and all predicted habit planes fell within a small grid near  $\{259\}_A$ . On the other hand the BM analysis with  $\delta=1.0108$  predicts a habit plane less than  $1\frac{1}{2}^\circ$  from the mean experimental one. However, the situation is less convincing when the orientation relationship is taken into consideration.

The theoretical orientation relationship can be obtained in the following manner. The invariant line is readily calculated as the intersection of the habit

plane (theoretical) and the shear plane. This is the eigenvector with unit eigenvalue of the matrix  $\delta RP$ . In addition, a plane with an invariant normal (Bowles & Mackenzie, 1954a),  $\mathbf{n}$ , which contains the directions of displacement due to the strains  $E$  and  $G^{-1}$ , can be determined since this normal must be orthogonal to the inhomogeneous shear direction and lie on the cone which describes the final position of unextended lines due to the strain  $\delta P$ . Or equivalently, the invariant normal can be found from the condition  $\mathbf{n}^T L = \mathbf{n}^T$ .<sup>\*</sup> The invariant line and invariant normal uniquely define the orientation relationship.

The rotation matrix,  $R$ , which describes the orientation relationship, is obtained by applying Euler's theorem to the following four vectors: the initial position of the invariant line,  $\mathbf{l}$ ; the position of  $\mathbf{l}$  due to the strain  $\delta P$ ; the initial position of the plane with the invariant normal,  $\mathbf{n}$ ; and the final position of this normal due to the strain  $(\delta P)^{-1}$ .

For the WLR case, the theoretical rotation matrix  $R$  is computed to be

$$R = \begin{pmatrix} 0.99665830 & 0.08004464 & 0.01628183 \\ -0.07772816 & 0.99063976 & -0.11221059 \\ -0.02511128 & 0.11057006 & 0.99355106 \end{pmatrix}.$$

For the BM analysis with  $\delta = 1.0108$ ,  $R$  is computed to be

$$R = \begin{pmatrix} 0.99758507 & 0.06243421 & 0.03042998 \\ -0.05801074 & 0.98991119 & -0.12926942 \\ -0.03819381 & 0.12719198 & 0.99114248 \end{pmatrix}.$$

The theoretical position of the (011) plane of the martensite is given by the position of the transformed  $(111)_A$  plane normal,

$$(011) = \frac{(111)_A (\delta RP)^{-1}}{|(111)_A (\delta RP)^{-1}|}.$$

In the WLR case,  $(011)_M$  is computed to be  $1'$  from  $(111)_A$ , which is at variance with the experimental orientation relationship. For the BM case with  $\delta = 1.0108$ ,  $(011)_M$  is computed to be  $11'$  from  $(111)_A$ ; however, the theoretical  $(011)_M$  plane does not lie between the habit plane and  $(111)_A$ , as experimentally observed. The use of a uniform dilation has been criticized previously on this basis (Wayman, 1961).

The theoretical position of the  $[11\bar{1}]_M$  direction can be calculated as

$$[11\bar{1}]_M^T = \frac{\delta RP [01\bar{1}]_M^T}{|\delta RP [01\bar{1}]_M^T|}.$$

In the WLR case  $[11\bar{1}]_M$  is found to be  $2^\circ 31'$  from  $[01\bar{1}]_A$  which is in reasonable agreement with the experimental  $[11\bar{1}]_M$  and  $[01\bar{1}]_A$  directions. However, as mentioned, the WLR analysis does not yield the correct habit plane or orientation between the close packed planes of the two structures. For the BM analysis,  $[01\bar{1}]_A$  is computed to be  $55'$  from  $[11\bar{1}]_M$ ,

in disagreement with the observed value,  $2^\circ 48'$ . Therefore, on the basis of the present data for the subject alloy and the assumption of  $\{112\}_M$  twinning, it appears that the situation may be more complicated than that given by theories assuming a uniform match of the two structures at the interface. A more general approach to the martensite crystallography problem involving a non-uniform dilation is presently being studied (C. M. Wayman, unpublished work; J. K. Mackenzie, private communication) and it is suggested that the incorporation of an additional anisotropic interface strain will give better agreement between theory and experiment, and in addition, account for 'sidewise' scatter in habit planes.

Although the inverse problem of deducing the elements of the lattice invariant shear system from the experimentally observed habit plane, orientation relationship, and lattice parameters is appealing in principle, there are certain difficulties which detract from the general usefulness of the inverse method just described. In reference to the invariant line strain and its factorization into two invariant plane strains Mackenzie (1960) and Bowles & Mackenzie (1954b) pointed out that the factorization is only possible when the orientation relationship satisfies certain geometrical conditions, which do not normally obtain owing to inevitable experimental errors. In fact, this means that the invariant line strain,  $L = \delta RP$ , is inaccurate because of uncertainties in the orientation relationship, *i.e.*, the matrix  $R$ . In other words, the invariant line as determined as an eigenvector of the matrix  $\delta RP$  does not always lie in the habit plane, and in such a case, the inverse method has no meaning. It will be shown below that this is a very significant point.

In this work, the Laue photograph on which the orientation relationship was based exhibited the following martensite reflections (in addition to those from the austenite): (011), (111), (012), (013), (132), and (213); the orthogonal martensite axes were also obtained from zones. The rotation matrix  $R$  can be determined by applying Euler's theorem to pairs of vectors and normals. The matrix  $R$  is such that normals and vectors in the Bain-strained position (designated  $(hkl)'$  and  $[uvw]'$ ) must be made coincident with the actual positions of the vectors and normals from the Laue photograph (designated  $(hkl)$  and  $[uvw]$ ).

A computer program was worked out so that orientation relation matrices  $R$  could be determined from pairs of vectors and normals. All possible pairs were considered. That is, for example,  $[010]$  and  $[010]'$ , were used along with  $[100]$  and  $[100]'$ ,  $(011)$  and  $(011)$ ,  $(012)$  and  $(012)'$ , *etc.* Thus, numerous  $R$  matrices were determined. The matrix  $P$  is known from the lattice parameters and therefore the invariant line strain  $L = \delta RP$  can be determined for each rotation matrix  $R$ . (This assumes that the lattice parameters are known to a more certain degree than the orientation relation-

\*  $T$  designates transpose.

ship.) The eigenvalues and eigenvectors of the matrices  $RP$  were then calculated by solving the characteristic equation. At least one of the three eigenvalues was near unity and the associated eigenvector determined the potentially invariant line (to be made invariant with the parameter  $\delta$ ).

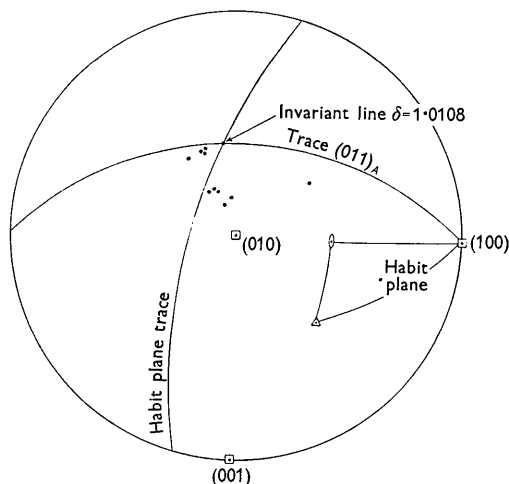


Fig. 4. Points on stereographic projection show various positions of the invariant line of the transformation. For each value of the matrix  $R$ , the invariant line was determined by solving the characteristic equation. The scatter is apparent.

Fig. 4 shows a stereographic projection on which are plotted the invariant lines determined by pairing vectors and normals with  $[010]_M$  and  $[010]_L$ . Also is shown the invariant line corresponding to  $\delta=1.0108$ , the value of  $\delta$  which gave best agreement between the observed and theoretical habit plane. It is seen that considerable scatter exists between the 'experimental' invariant lines. Bearing in mind that all of these invariant lines were determined from one Laue photogram, it is clear that even one determination of the orientation relationship is not of itself entirely consistent. In addition, for each of these invariant lines, the value of the parameter delta was determined from the condition  $\delta\lambda=1$ . These values were all unreasonably large ( $\delta>1.025$ ), and there was much scatter between individual values. Therefore, on the basis of the observed data it is apparent

that the invariant line strain is an experimentally inaccurate quantity. Mackenzie (1957) has suggested a method for minimizing experimental errors in orientation relationships; this amounts to a least-squares fitting of the elements of the matrix  $R$ , but does not necessarily ensure that the adjusted invariant line will lie in the habit plane.

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