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A GENERALISED LATTICE CORRESPONDENCE FOR PHASE TRANSFORMATIONS

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UNA CORRESPONDENCIA DE REDES GENERALIZADA PARA TRANSFORMACIONES DE FASE

por

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Resumen

A cada átomo en una dada posición de la fase matriz se le asigna una cierta probabilidad de que ocupará, una vez producida la transformación, una dada posición en la fase producto. Este enfoque probabilístico de los movimientos atómicos permite definir un vector $_{o}\vec{k}$ que es un promedio pesado de todos los sitios en la fase original cuyos átomos tienen una probabilidad finita de ocupar una posición dada en la fase transformada.

Para transformaciones que generan una deformación homogénea macroscópica, se define una correspondencia generalizada que incorpora la posibilidad de un cierto grado de independencia de los movimientos atómicos. Este modelo se usa para explicar la cristalografía de la ferrita Widmanstätten. A partir de este ejemplo se concluye que, si se admite una correspondencia generalizada para transformaciones que producen un cambio de forma de tipo martensítico, 1) una microestructura puede ser no necesaria para describir la totalidad de los movimientos atómicos, y 2) la hipótesis de distorsiones adicionales en el plano de hábito es innecesaria.

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Abstract

Each atom in a given position of the matrix phase is assigned a certain probability that it will occupy, upon transformation, a given site in the product phase. This probabilistic view of the atomic movements permits to define a vector $_{o}\vec{k}$ which is a weighted average of all the sites in the parent phase the atoms at which have a finite probability of occupying a given position in the transformed phase.

For transformations generating a macroscopic homogeneous deformation, a generalised correspondence is defined that incorporates the possibility of a certain degree of independence of atomic movements. This approach is used to explain the crystallography of the Widmanstätten ferrite. Out of this example it is concluded that if a generalised correspondence is assumed for transformations producing a martensitic type of shape change, 1) a microstructure may be not necessary for describing the total atomic displacements, and 2)the hypothesis of additional distortions in the habit plane is unnecessary.

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INTRODUCTION

One of the main features of a first order phase transformation involving two solid phases is that the new phase grows strongly (mechanically) constrained by the surrounding medium (matrix). In the product phase, atomic interactions differ from those in the parent crystal. Hence, in general, a change of shape of the original unit cell and/or a change of volume per atom occur on transformation. These two changes must be counterbalanced, and therefore they condition the growth of the new phase.

Our knowledge of the mechanisms of compensation of the lattice shape and volume changes is derived from the observation of samples that are very large compared to the size of a single unit cell; the experimental measurements thus relate to the average behavior of a very large number of atoms, whose individual behavior may, however, depart considerably from the average. Hence, a natural approach to the understanding of phase transformation phenomena is to consider them in terms of the average atomic behavior and to analyse separately how this average can be accounted for in terms of the behavior of the individual atoms. This approach cannot rely on the crystallographic features of a transformation alone, because they relate to static observations. Instead, the fact that a phase transformation is a

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dynamic process must be taken into consideration.

In this paper, a first analysis of the physical concepts involved in the study of the possible mechanisms for compensating the shape and volume changes of the unit cell is attempted. Transformations involving no changes of composition are considered; nevertheless, many of the concepts here developed may be straightway applied to certain cases where such changes do take place.

THE UNCONSTRAINED PRODUCT CRYSTAL

The initial (parent) and final (product) lattices will be described by means of the reference bases $\mathcal{I}$ and $\mathcal{F}$, respectively. For any given orientation relationship between the two lattices, a vector $\vec{v}$ referred to the basis $\mathcal{F}$ is related to the same vector referred to the basis $\mathcal{I}$ through the following equation

$$[\mathcal{F} \,;\, v] = (\mathcal{F}\, T\, \mathcal{I}) \quad [\mathcal{I} : v] \qquad (1)$$

where T is a non singular matrix. The matrix T may be written as

$$T = RT_{m} \qquad (2)$$

where R is a rotation and T_{m} is a matrix that changes the metric.

Let $^{\mathcal{I}}\vec{k}$ and $^{\mathcal{F}}\vec{k}$ denote lattice vectors in the initial and final lattices[**]. One basic question in the study of any solid-

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(*) In the following, the notation introduced by Mackenzie and Bowles (1) will be used.

(**) Hereafter, the case of monoatomic primitive cells will be referred to.

solid phase transformation relates to which is the site ${}^F\vec{k}$ in the new phase that an atom located at ${}^I\vec{k}$ in the matrix, will occupy. In this respect, it may generally be stated that there exists a certain probability $p_{{}^Ik\,{}^Fk}$ that an atom (or vacancy) occupying the position ${}^I\vec{k}$ will after transformation be at ${}^F\vec{k}$. If the system is conservative,

$$\sum_{{}^I\vec{k}} p_{{}^Ik\,{}^Fk} = \sum_{{}^F\vec{k}} p_{{}^Ik\,{}^Fk} = 1$$

for every ${}^F\vec{k}$ and ${}^I\vec{k}$ site, respectively.

The first problem being raised in this analysis is to properly define the initial and final atom lattice sites since, although the description to be made is formally static, it is of capital importance to consider the dynamic character of a phase transition. In this respect, the atoms both in the matrix and in the product crystal continuously change positions because of the general occurrence of self diffusion. Thus, an atom can diffuse in the matrix from its position ${}^I\vec{k}$ onto ${}^I\vec{k}'$, then move across the interface (including a possible migration inside it) from ${}^I\vec{k}'$ onto ${}^F\vec{k}'$, and finally diffuse in the new phase onto ${}^F\vec{k}$. Each one of these processes may be considered to have a certain probability of occurrence. Then, the probability that an atom at ${}^I\vec{k}$ will, after transformation, be at ${}^F\vec{k}$ is

$$p_{{}^Ik\,{}^Fk} = \sum_{{}^I\vec{k}',\,{}^F\vec{k}'} p_{{}^Ik\,{}^Ik'} \; p_{{}^Ik'\,{}^Fk'} \; p_{{}^Fk'\,{}^Fk} \qquad (3)$$

where the vectors ${}^I\vec{k}'$ and ${}^F\vec{k}'$ denote positions on surfaces, these surfaces being time dependent since they are adjacent to a moving interface. Each probability in the r.h.s. of equation (3) accounts for the above enunciated processes; in particular, $p_{{}^Ik'\,{}^Fk'}$ must depend upon the nature of the interface.

The ${}^{I}\vec{k}'$ vectors for a given ${}^{I}\vec{k}$ such that $p_{{}^{I}k\,{}^{I}k'} \neq 0$ are determined by the diffusivity of the corresponding atom species in the matrix and by the time available for diffusion. A similar statement applies in connection with the ${}^{F}\vec{k}'$ vectors for a given ${}^{F}\vec{k}$ in the product phase such that $p_{{}^{F}k\,{}^{F}k} \neq 0$. Therefore, a criterion for bounding the diffusion times must be given. First, it appears convenient to define steady state growth conditions. These conditions are such as to allow the new phase to grow under a constant elastic field (due to transformation strains), and in the case of transformations involving changes of composition, under a constant solute field as well. In steady state, the diffusion times available both in the matrix and in the product will be assumed to be of the order of a/V, where a is a minimum distance the interface travels (say, one interplane distance) and V is the transformation rate. The time available for diffusion in the interface is of the order of d/V, where d is the interface width.

If an atom (or vacancy) located at ${}^{I}\vec{k}$ in the initial lattice moves onto ${}^{F}\vec{k}$ after transformation, the two lattice vectors are related as follows

$$[F\ ;\ {}^{F}k] = (F\ P^{{}^{I}k\,{}^{F}k}\ I)[I;\ {}^{I}k] \tag{4}$$

where $P^{{}^{I}k\,{}^{F}k}$ is in general a function of both ${}^{I}\vec{k}$ and ${}^{F}\vec{k}$. If the assumption is made that there exists a certain probability that an atom at ${}^{I}\vec{k}$ will move, upon transformation, onto ${}^{F}\vec{k}$, then each ${}^{F}\vec{k}$ lattice vector can be uniquely associated with one vector

$$[I\ ;\ {}_{0}k] = \sum_{{}^{I}\vec{k}} p_{{}^{I}k\,{}^{F}k}\,[I\ ;\ {}^{I}k] \tag{5}$$

${}_{0}\vec{k}$ being a weighted average of all the I lattice sites the atoms at which have a finite probability of occupying ${}^{\mathcal{F}}\vec{k}$. Equation (4) may now be generalised as follows

$$[\mathcal{F} ; {}^{\mathcal{F}}k] = (\mathcal{F}\, P^{{}^{o}k\,{}^{\mathcal{F}}k}\, \mathcal{I})\, [\mathcal{I} ; {}_{0}k] \qquad (6)$$

Here, $P^{{}^{o}k\,{}^{\mathcal{F}}k}$ is in general a function of ${}_{0}\vec{k}$ and ${}^{\mathcal{F}}\vec{k}$. The ${}_{0}\vec{k}$ vectors do certainly not describe a real atomic arrangement in the matrix. Equation (5) has a statistical character and establishes the effective atomic arrangement which - in the dynamic process of a phase transformation where a very large number of atoms is involved - the F lattice should be related with. Whenever the points whose positions are described by the vectors ${}_{0}\vec{k}$ are arranged in a crystal lattice, this will be denoted as the D lattice in order to emphasize its dynamic signification. In this approach, the displacement vector referred to the basis $\mathcal{I}$, for a given ${}^{\mathcal{F}}\vec{k}$, is

$$\begin{aligned}[\mathcal{I} ; u ({}^{\mathcal{F}}\vec{k})] &= \left\{ (\mathcal{I}\, T\, \mathcal{F})(\mathcal{F}\, P^{{}^{o}k\,{}^{\mathcal{F}}k}\, \mathcal{I}) - (\mathcal{I}\, I\, \mathcal{I}) \right\} [\mathcal{I} ; {}_{0}k] \\ &= \sum_{{}^{\mathcal{I}}\vec{k}} p_{{}^{\mathcal{I}}k\,{}^{\mathcal{F}}k} \left\{ (\mathcal{I}\, T\, \mathcal{F})(\mathcal{F}\, P^{{}^{o}k\,{}^{\mathcal{F}}k}\, \mathcal{I}) - (\mathcal{I}\, I\, \mathcal{I}) \right\} [\mathcal{I} ; {}^{\mathcal{I}}k]\end{aligned} \qquad (7)$$

These displacements provide information on the macroscopic change of shape when the crystal grows free of constraints.

RELATIONSHIP BETWEEN THE UNCONSTRAINED AND THE CONSTRAINED PRODUCT CRYSTALS

Inasmuch as the interface is the boundary surface between the transformed phase and the parent one, it may only be realized when the new phase grows mechanically connected with the matrix. But this is tantamount to establishing the corresponding constraints. When the constraints are introduced, the shape of the region in the matrix which has transformed must necessarily coincide with the shape of the product crystal, provided there are no free surfaces. This shape requirement puts forward the necessity of properly choosing the probability distribution.

Consider first the case of a conservative system where there is no volume change. The probabilities $p_{s_k r_k}$ may always be chosen such that no macroscopic shape change occurs upon transformation, and then the constrained and the unconstrained situations are identical. Nevertheless, the mechanisms thus selected via the probabilities may be non feasible from a kinetic standpoint (see, for instance, Appendix I). In general, the mechanisms of compensation of the shape change of the unit cell require the existence of an elastic field for a realistic probability distribution to be defined. This means that in the unconstrained condition the surface of the transformed region in the matrix and that of the product crystal do not coincide. Instead, they differ so that when the product crystal is actually immersed in the matrix, the elastic field necessary for accounting for this shape difference is generated. It is therefore concluded that a given probability distribution determines the elastic field which develops when the new crystal grows under its actual constraints.

With the exception of very small particles where the interface free energy may become important, it may be reasoned that this elastic field should be a minimum so as to allow the transformation to proceed at its maximum possible rate. This implies the choice of a probability distribution that minimizes the elastic stresses built up during transformation in a way compatible with the atomic mobility under given constraints. This criterion does of course not preclude the occurrence of different growth morphologies and kinetics in the same material and even at the same temperature. Eventually, plastic deformation may become necessary for accommodating shape differences either during growth or after the process of transformation has been interrupted.

If there is volume change per atom, an adequate choice of the probability distribution which produces a minimization of the elastic field, and thus an optimum compensation of the overall volume change, may allow an analysis of the real case through the unconstrained one (2). Another instance where the two conditions might be related is that of a non conservative system, e.g. the interface may operate either as a vacancy source or as a sink. If $p_{{}^{I}k'\,{}^{F}k'}$ is the probability that a vacancy at ${}^{I}\vec{k}'$ will, after transformation, be at ${}^{F}\vec{k}'$ (${}^{I}\vec{k}'$ and ${}^{F}\vec{k}'$ denote positions adjacent to the interface)

$$\sum_{{}^{I}\vec{k}'} p_{{}^{I}k'\,{}^{F}k'} \gtrless 1 \qquad (8)$$

where the upper inequality applies when the interface behaves as a sink and the lower one applies when the interface behaves as a source. In the first case, there is a net vacancy flow from the interface towards the matrix free surface, while in the second one this flow is reversed. In this instance, an elastic field driving the vacancy chemical potential must clearly exist. Again, for the volume partial or total compensation to occur, plastic deformation may eventually become operative for the real crystal to grow.

The concept of a transformation interface for the unconstrained product crystal may now be introduced in the framework of the preceding analysis. An interface will be said to be fully coherent when for each ${}^{F}\vec{k}'$ vector there is one and only one ${}^{I}\vec{k}'$ vector such that $p_{{}^{F}k'\,{}^{F}k'} = 1$, and zero for any other ${}^{I}\vec{k}'$ vector. An immediate property that follows from this definition is that a coherent interface cannot operate as a vacancy source or sink. A fully incoherent interface is defined in the limit situation where for any defined position of it the probabilities $p_{{}^{F}k', {}^{F}k'}$ have the same (non zero) value for every ${}^{F}\vec{k}'$, ${}^{F}\vec{k}'$ pair. In Appendix I it is demonstrated that this particular probability distribution entails that the stored elastic energy due to the shape change of the unit cell is zero, and that all the ${}^{F}\vec{k}$ vectors are associated - through equation (5) - with only one ${}_{0}\vec{k}$. If ${}_{0}\vec{k}$ is chosen to be the nul vector, the matrices $P^{{}_{0}k\,{}^{F}k}$ should all be singular; hence, equations (6) and (7) are not valid in this case. It should be pointed out that, while other definitions of an interface are static, the present one takes into account mainly the dynamic character of a transformation, which is implicit in the probability distribution.

HOMOGENEOUS STRAIN. A GENERALISED CORRESPONDENCE

By analogy with the theory of elasticity, a phase transformation will be said to generate an homogeneous deformation when the matrices $P^{{}_{0}k\,{}^{F}k}$ - defined for the unconstrained condition-are independent of both ${}_{0}\vec{k}$ and ${}^{F}\vec{k}$, i.e.,

$$[\mathcal{F} ; {}^{F}k] = (\mathcal{F}\ P\ \mathcal{I})\ [\mathcal{I} ; {}_{0}k] \qquad (9)$$

Obviously in this case, the sites described by the vectors ${}_{0}\vec{k}$ are arranged in a crystal lattice.

Let $\mathcal{D}$ be a basis in D and suppose that the relation between $\mathcal{I}$ and $\mathcal{D}$ is given by

$$[\mathcal{D} ; {}_{0}k] = (\mathcal{D}\ J\ \mathcal{I})\ [\mathcal{I} ; {}_{0}k] \qquad (10)$$

so that (9) may be written

$$\left[{}_{F} \; ; \; {}^{F}k \right] = ({}_{F} \, C \, {}_{D}) \left[{}_{D} \; ; \; {}_{0}k \right] \qquad (11)$$

where

$$({}_{F} \, C \, {}_{D}) = ({}_{F} \, P \, {}_{I}) ({}_{I} \, J \, {}_{D}) \qquad (12)$$

The strain associated with the correspondence C is

$$({}_{D} \, S \, {}_{D}) = ({}_{D} \, J \, {}_{I}) ({}_{I} \, T \, {}_{F}) ({}_{F} \, C \, {}_{D}) \qquad (13)$$

and the displacement vector for any given ${}^{F}\vec{k}$ vector is

$$\left[{}_{D} \; ; \; u \, ({}^{F}\vec{k}) \right] = \left\{ ({}_{D} \, S \, {}_{D}) - ({}_{D} \, I \, {}_{D}) \right\} \left[{}_{D} \; ; \; {}_{0}k \right] \qquad (14)$$

Substituting now equation (5) for $\left[{}_{I} \; ; \; {}_{0}k \right]$ in (9) yields

$$\left[{}_{F} \; ; \; {}^{F}k \right] = ({}_{F} \, P \, {}_{I}) \sum_{{}^{I}\vec{k}} p_{{}^{I}k \, {}^{F}k} \left[{}_{I} \; ; \; {}^{I}k \right] \qquad (15)$$

This equation describes a generalised correspondence between the I and the F lattice vectors. While $({}_{F} \, C \, {}_{D})$ is a matrix which has integral elements and determinant ± 1 provided the bases ${}_{D}$ and ${}_{F}$ both define primitive unit cells (1), this is not always the case for the matrix $({}_{F} \, P \, {}_{I})$.

A very important example of a transformation generating an homogeneous deformation is that of martensite. In this case, the homogeneous deformation that accompanies the formation of the product phase may be described by an invariant plane strain. In the phenomenological theories (3,1) a one to one correspondence between the I and the F lattice vectors is assumed. Namely, in the present formulation,

$$p_{{}^{I}k' \, {}^{F}k'} = 1$$

But this strain alone cannot - in most cases - describe the total atomic displacements and hence the necessity of an additional inhomogeneous strain. Moreover, in many applications of the phenomenological theories it has been necessary to assume that the invariant plane strain condition is met apart of either a uniform dilatation (4,5) or an anisotropic distortion (6) in the habit plane.

If a generalised correspondence is assumed, the invariant plane strain has to be associated with the correspondence (ꜰ C ᴅ) that relates the D and the F lattice vectors. Thus (D lattioe) planes are transformed into planes, and straight lines into straight lines, since the shape deformation is macroscopically homogeneous. But because of the probabilistic nature of the correspondence (ꜰ P ɪ), average (I lattice) planes and straight lines are respectively transformed into defined planes and directions. The width of the region in the I lattice having that average plane or line clearly depends on the characteristics of the probability distribution.

Two fundamental questions arise in the framework of the concept of a generalised correspondence when a transformation produces an homogeneous deformation that can be described in terms of an invariant plane strain:

1) Is it always nacessary the existence of a microstructure?
2) Is it necessary to introduce a distortion - either isotropic or anisotropic - in the habit plane ?

An attempt to answer these two questions is made for the case analysed in the next section.

THE AUSTENITE TO WIDMANSTÄTTEN FERRITE TRANSFORMATION

The morphological features of the Widmanstätten ferrite are similar to those of martensite with respect to the shape change of the transformation, which is an invariant plane strain (7). However, there is no conclusive experimental evidence - up to now - of the existence of a microstructure in the ferrite plates. Two possibilities can be thought of, viz. either this microstructure cannot be observed by the available experimental methods, or it does not exist at all. In the latter case, it may be suggested that a certain independence of the individual atomic movements might substitute for the necessity of a microstructure. Considering the temperature range at which the ferrite plates form, this assumption does not seem unreasonable.

The experimentally observed orientation relationship is very close to that of Kurdjumov-Sachs, namely

$$(111)_\gamma // (101)_\alpha \quad \text{and} \quad [1\bar{1}0]_\gamma // [11\bar{1}]_\alpha$$

for the variant of the correspondence considered by Watson and McDougall (8). Consider first the case where the generalised correspondence $({}^{F}P\,{}^{I})$ associates every F lattice vector of a $(101)_\alpha$ plane with I vectors of only one $(111)_\gamma$ plane. Thus, $\sum_{{}^{I}\vec{k}} p_{{}^{F}k\,{}^{I}k} = 1$ where all the ${}^{I}\vec{k}$ vectors relate to sites of the same $(111)_\gamma$ plane. In fig. 1 the sites of both planes are drawn superimposed. It can be seen that every Fe atom site of the α-phase is mostly located inside a triangle whose vertices are the three nearest Fe atom sites of the γ-phase.

Let the probability distribution that any given α site be occupied by any one of the atoms at those three γ lattice positions be proportional to the distance from the α site to the side of the triangle opposite to the γ site considered. Assuming that no atomic interchange takes place, the constant of proportionality is the reciprocal of the height of the γ-triangle in question. This choice of the probability distribution - pictured in fig. 2a - obviously yields a D plane whose sites coincide with those of a $(101)_\alpha$ plane. This distribution was calculated for 1800 sites in each plane (α and γ); the overall results are independent of translations of one plane relative to the other. Representative results of the probability distribution are given in Table I. The lattice parameters that have been used (Table II) are those that correspond to the assumption that the transformation occurs between phases of the equilibrium compositions at the transformation temperature (700 °C), in the vicinity of the interface.

In Table I it can be seen that the average of $p_{\gamma_k} = \sum_{F_k} p_{\gamma_k F_k}$ - where the sum is carried over all the $^{F}\vec{k}$ vectors of one $(101)_\alpha$ plane - equals the ratio of the density of sites of the D plane to that of the γ plane (see Appendix II). It can also be noticed that the distribution of p_{γ_k} is non uniform in a $(111)_\gamma$ plane. Since the system being considered is conservative, p_{γ_k} should equal 1. This means that there is a finite probability for an atom at $^{\gamma}\vec{k}$ to go onto different α planes, this probability depending on the particular $^{\gamma}\vec{k}$ vector. This is in contradiction with the above assumed generalised correspondence.

Consider then the case where a further independence of the individual atomic movements is allowed such that the vectors $^{\gamma}\vec{k}$ for which $p_{\gamma_k F_k} \neq 0$ denote sites of two adjacent $(111)_\gamma$ planes, and let the probability distribution be as pictured in Fig. 2b. The correspondence matrix $(F\ C\ D)$ is the identity matrix provided the bases F and D are identical. The average of p_{γ_k} is again different from 1, this result being a consequence of the volume change of the transformation (- 7.37 ‰). This difficulty is easily overcome for instance by assuming that the $(101)_D$ planes are spaced so that the volume per "atom" of the D lattice equals that of the γ lattice, and thus the correspondence $({}_F C {}_D)$ is associated with a compresion normal to the $(101)_D$ planes. But still, the distribution of p_{α_k} is non-uniform, the standard deviation being $\sigma = 0.018$.

Under the preceding assumptions of restricted independence of individual atomic movements - no atomic interchange being allowed - there are two plausibilities to overcome this contradiction. One is to assume that there are extended distortions in D regions which are related with γ regions of equiprobability (of low or high value of p_{α_k} compared to the average), namely that the $(101)_D$ is similar to a $(101)_\alpha$ plane inhomogeneously distorted. The other one is to assume that there is an homogeneous strain - which in principle might not be unique, necessarily - associated with the correspondence $({}_F C {}_D)$. The problem then centres in finding the D lattice (or lattices) which homogeneously deformed will yield the α lattice under the condition that p_{α_k} be uniform through any $(111)_\gamma$ plane.

As mentioned above, the Widmanstätten ferrite produces a shape deformation that can be described by an invariant plane strain. The experimental results of reference (8) will next be used by assuming that this strain is associated with the correspondence between the D and the α lattice vectors, and that there is no complementary strain. Thus

$$({}_D S {}_D) = ({}_D J {}_\alpha)\,({}_\alpha S_\varepsilon {}_\alpha)\,({}_\alpha J {}_D) \qquad (16)$$

where

$$S_\varepsilon = I + m_1 d_1 p_1' \qquad (17)$$

S_ε is the experimentally determined strain, m_1 and d_1 are respectively the magnitude and the unit vector in the direction of the strain, and p_1 is the normal to the habit plane. Then, from equation (9)

$$\left[\,I\ ;\ {}_{0}k\,\right] = (I\ S_{\varepsilon}^{-1}\ I)\ \left[\,I\ ;\ {}^{\varepsilon}k\,\right] \tag{18}$$

where

$$S_{\varepsilon}^{-1} = I - m_1 d_1 p_1' \,/\, (\,1 + m_1 p_1' d_1\,) \tag{19}$$

The relevant data given in ref. (8) are reproduced here in Table II. First, the orientation relationships for all the cases may be derived by applying the condition that the habit plane be undistorted. Thus (see Appendix III)

$$\sin \lambda = m_1 \sin(\psi - \lambda)\, |d_{12}| / 0.9926 \tag{20}$$

where λ is the angle between the α and γ planes, ψ is the angle between the $(111)_\gamma$ and the habit plane, and d_{12} is the component of the unit vector $\vec{d}_1$ in the $[111]_\gamma$ direction. The results are given in the first column of Table III. Next, since the D lattice is known, the probability distributions are easily calculated by using the same criterion as illustrated in fig. 2a. The details of the calculation - made for 1800 sites - are given in Appendix III. Representative results are shown in Table IV, while the average of p_{r_k} for all the cases presented in Table II, are given in Table V. The distribution of sums of probabilities is notoriously uniform in all the cases, although still $p_{r_k} \neq 1$.

Watson and McDougall have assumed that the invariant plane strain on the habit plane accounts for all of the volume change of the transformation. This implies that the volume per "atom" of the D lattice must equal that of the γ lattice. If p_{r_k} were equal to 1, the D planes that transform into $(101)_\alpha$ planes would coincide in space with the $(111)_\gamma$ planes, and the orientation relationship necessary for keeping the habit plane undistorted would differ from that of Kurdjumov-Sachs by

$$\lambda = tg\,\psi\ (1 - t_\alpha / t_\gamma) \qquad (21)$$

where t_α and t_γ are respectively the $(101)_\alpha$ and the $(111)_\gamma$ spacings (6). The angles calculated with equation (21) are different from those given in Table III. On the other hand, in Table V it can be seen that for the cases reported in ref. (8) $p_{z_k} \neq 1$. This result indicates that the appropriate probability distribution should be that pictured in fig. 2b.

The assumed generalised correspondence associates lattice vectors of two adjacent $(111)_\gamma$ planes with those of one $(101)_\alpha$ plane. Hence, the D related planes must be parallel to the $(111)_\gamma$ planes. By applying now the criterion of fig. 2b, it should be obtained that (see Appendix III)

$$p_{z_k}\ (2\,t_\gamma - t_\alpha)\ /\ t_\gamma = 1 \qquad (22)$$

Otherwise, equation (22) may be used to derive the angle λ, provided p_{z_k} is known. The results of this calculation are given in the second column of Table III, showing an excellent agreement with the previously calculated values.

The crystallography of the Widmanstätten ferrite has been explained in a consistent manner in the framework of a generalised correspondence. The homogeneous character of the shape deformation has been shown to be properly described in terms of an invariant plane strain on the habit plane. It has further been shown that in principle no microstructure is necessary in this transformation for accommodating the shape deformation, and that the scatter of experimental data can be accounted for.

CONCLUSION

The correspondence between lattice vectors of parent and product is one of the most important physical concepts of the phenomenological theories of the transformations that generate an invariant plane strain. In this work an attempt has been made for demonstrating that this concept does not necessarily imply that atoms move in a strictly cooperative manner. E.g., if a certain degree of independence of the individual atomic movements be allowed, the essentials of the concept of correspondence are preserved.

The macroscopic character of the overall shape change allows a description of a phase transformation in statistical terms; this fact is the foundation of the generalised correspondence. A successful analysis of the crystallography of the Widmanstätten ferrite has been accomplished, thus rendering support to the approach here presented.

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TABLE I

DISTRIBUTION OF THE PROBABILITIES $p_{s_k} = \sum_{r_k} p_{s_k r_k}$

(The labels i and j refer to the relative positions of the I lattice points along the $(\bar{1}\bar{1}2)_s$ and the $(\bar{1}10)_s$ directions, respectively)

j i	1	2	3	4	5	6	7	8	9	10
1	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975
2	0.975	0.975	0.975	0.975	0.975	0.955	0.944	0.944	0.944	0.944
3	0.944	0.944	0.944	0.944	0.964	0.975	0.975	0.975	0.975	0.975
4	0.975	0.975	0.975	0.975	0.975	0.975	0.990	1.005	1.005	1.005
5	0.975	0.988	1.005	1.005	1.005	1.005	0.989	0.975	0.975	0.975
6	1.005	1.005	0.992	0.975	0.975	0.975	0.975	0.975	0.975	0.975
7	0.975	0.975	0.975	0.975	0.975	0.962	0.944	0.944	0.944	0.944
8	0.944	0.944	0.944	0.944	0.944	0.957	0.975	0.975	0.975	0.975
9	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975
10	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975	0.975

Average : $\bar{p}_{s_k} = .977$ Standard deviation : $\sigma = .019$

TABLE II

HABIT PLANE AND SHAPE STRAIN DETERMINATIONS (FROM REF. 8)

(All the results are given relative to the γ basis)

Plate	Habit plane	Shape strain	
		d_1	m_1
1	(0.4444 0.3635 0.8187)	[-0.8762 0.3956 0.2750]	0.360
2	(0.4467 0.3689 0.8151)	[-0.9022 0.2613 0.3432]	0.274
3	(0.4772 0.4027 0.7811)	[-0.8417 0.4828 0.2418]	0.402
4	(0.4681 0.3771 0.7992)	[-0.8764 0.3675 0.3112]	0.321
5	(0.5056 0.4402 0.7420)	[-0.8097 0.5501 0.2045]	0.476

Lattice parameters : Ferrite (0% carbon) a' = 2.897 Å

Austenite (0.8% carbon) a = 3.659 Å

TABLE III

ORIENTATION RELATIONSHIPS

Plate	λ (Equation 20)	λ (Equation 22)
1	49′	49′
2	53′	57′
3	26′	27′
4	38′	38′
5	12′	11′

TABLE IV

DISTRIBUTION OF THE PROBABILITIES $p_{s_k} = \sum_{\epsilon_k} p_{s_k \epsilon_i}$
FOR PLATE N° 3

j / i	1	2	3	4	5	6	7	8	9	10
1	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995
2	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995
3	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995
4	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995
5	0.987	0.987	0.992	0.995	0.995	0.995	0.995	0.995	0.995	0.995
6	0.995	0.995	0.995	0.991	0.987	0.987	0.987	0.987	0.987	0.987
7	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995
8	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995
9	1.011	1.001	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995
10	0.995	1.001	1.011	1.011	1.011	1.011	0.997	0.995	0.995	0.995

TABLE V

PARAMETERS OF THE p_{I_k} DISTRIBUTION

Plate	Average $\bar{p}_{I_k}$	Standard Deviation σ
1	1.009	0.005
2	1.017	0.008
3	0.996	0.005
4	1.003	0.005
5	0.983	0.004

TABLE VI

SUMMARY OF THE COMPONENTS OF THE VECTOR d AND OF THE ANGLES USED IN THE CALCULATION OF THE D LATTICE

Plate	$\vec{d}_{111}$ (relative to the γ-basis)	$\lvert\vec{d}_{111}\rvert$	$\lvert\vec{d}_{12}\rvert$	Ψ	φ	θ
1	[-0.8077 0.4641 0.3435]	0.9928	0.1187	20° 5′	9° 35′	25° 4′
2	[-0.8030 0.3605 0.4424]	0.9851	0.1719	19° 42′	9° 23′	33° 21′
3	[-0.8027 0.5218 0.2808]	0.9977	0.0676	16° 28′	10° 46′	20° 29′
4	[-0.8105 0.4334 0.3771]	0.9934	0.1141	18° 18′	11° 52′	27° 39′
5	[-0.7913 0.5685 0.2229]	0.9995	0.0318	12° 58′	11° 50′	15° 57′

FIGURE CAPTIONS

Fig. 1 . Atomic configurations of the $(111)_\gamma$ and the $(101)_\alpha$ planes, superimposed in accordance with the Kurdjumov-Sachs orientation relationship.

Fig. 2 . Diagram illustrating the probability distribution that yields the generalised correspondence associating the lattice vector ${}^{F}\vec{k}$ with:

a) the vectors ${}^{I}\vec{k}_1$, ${}^{I}\vec{k}_2$, ${}^{I}\vec{k}_3$;

b) the vectors ${}^{I}\vec{k}_1$, ${}^{I}\vec{k}_2$, ${}^{I}\vec{k}_3$, ${}^{I}\vec{k}_4$, ${}^{I}\vec{k}_5$ and ${}^{I}\vec{k}_6$.

Fig. 3 . a) Diagram showing the trace of the habit plane on the $(111)_\gamma$ plane.

b) A view normal to the trace of the habit plane, showing the relative positions of the γ , D and α related planes.

APPENDIX I

THE CONDITION FOR ZERO MACROSCOPIC SHAPE CHANGE

If in the unconstrained situation the probability distribution relating atom sites adjacent to the interface at times differing by d/V - d being the interface width for the constrained crystal and V the instantaneous growth velocity - are such that $p_{{}^{I}k',{}^{F}k'} \neq 0$, all these probabilities having the same value for all the ${}^{I}\vec{k}'$, ${}^{F}\vec{k}'$ pairs, and the volume change is zero, then : i) the interface advances at the same rate in every place maintaining its shape, and ii) the interface is spherical.

First assume that the interface has any given shape. There being no volume change, the system is conservative. If the interface advanced at a non uniform rate, then one could think of at least one ${}^{F}\vec{k}'$ which corresponds to, say, two different positions of the interface in another region. The probabilities $p_{{}^{I}k'\,{}^{F}k'}$ for this ${}^{F}\vec{k}'$ site would be different from those related with other ${}^{F}\vec{k}'$ sites. For, after the interface has advanced somewhere else, the ${}^{F}\vec{k}'$ position in question becomes related with an increased number of ${}^{I}\vec{k}'$ positions. This cannot be the case, and hence the interface must advance at a uniform rate thus maintaining its shape.

Inasmuch as the interface advances at a uniform rate - although not necessarily constant - there can be no crystallographic anisotropies affecting the growth kinetics. Therefore the interface must be spherical. This being the shape no matter what the orientation relationship between the two crystals be, there is no macroscopic shape change . Consequently, as long as the volume change is zero, there is no elastic field built up during the transition.

Let the position of any I lattice point be given by its coordinates ${}^{I}k_i$ with respect to some origin and a set of base vectors I. Then, ${}^{I}\vec{k}$ may be written as

$$ {}^{I}\vec{k} = \vec{k}_1 + {}^{I}\vec{k}'' $$

where $\vec{k}_1$ denotes the position of the centre of the spherical transformed region. From equation (5) it follows that

$$ \left[I \; ; \; {}_{0}k \right] = \left[I \; ; \; k_1 \right] + \sum_{{}^{I}k''} p_{{}^{I}k''\,{}^{F}k} \left[I \; ; {}^{I}k'' \right] \qquad \text{(A1)} $$

Taking now into account equation (3) and that, there being no elastic stresses

$$ \sum_{{}^{I}k'} p_{{}^{I}k\,{}^{I}k'} \left[I ; {}^{I}k \right] = \left[I \; ; {}^{I}k' \right] $$

equation (A1) becomes

$$ \begin{aligned} \left[I \; ; \; {}_{0}k \right] &= \left[I \; ; \; k_1 \right] + \sum_{{}^{I}k',\,{}^{F}k'} p_{{}^{I}k'\,{}^{F}k'} \; p_{{}^{F}k'\,{}^{F}k} \left[I ; {}^{I}k' \right] \\ &= \left[I ; \; k_1 \right] \end{aligned} $$

since the system is conservative. Thus, if $\vec{k}_1$ is chosen as the nul vector, the matrices $P^{{}^{I}k\,{}^{F}k}$ are all singular.

From a physical point of view, this particular probability distribution describes a process where the transformation velocity is much lower than the diffusion rate inside the interface. That is, if the radius of the product crystal is r, then - using a random walk approximation -

$$ \frac{\pi^2 r^2}{4 D_i} \ll \frac{d}{V} $$

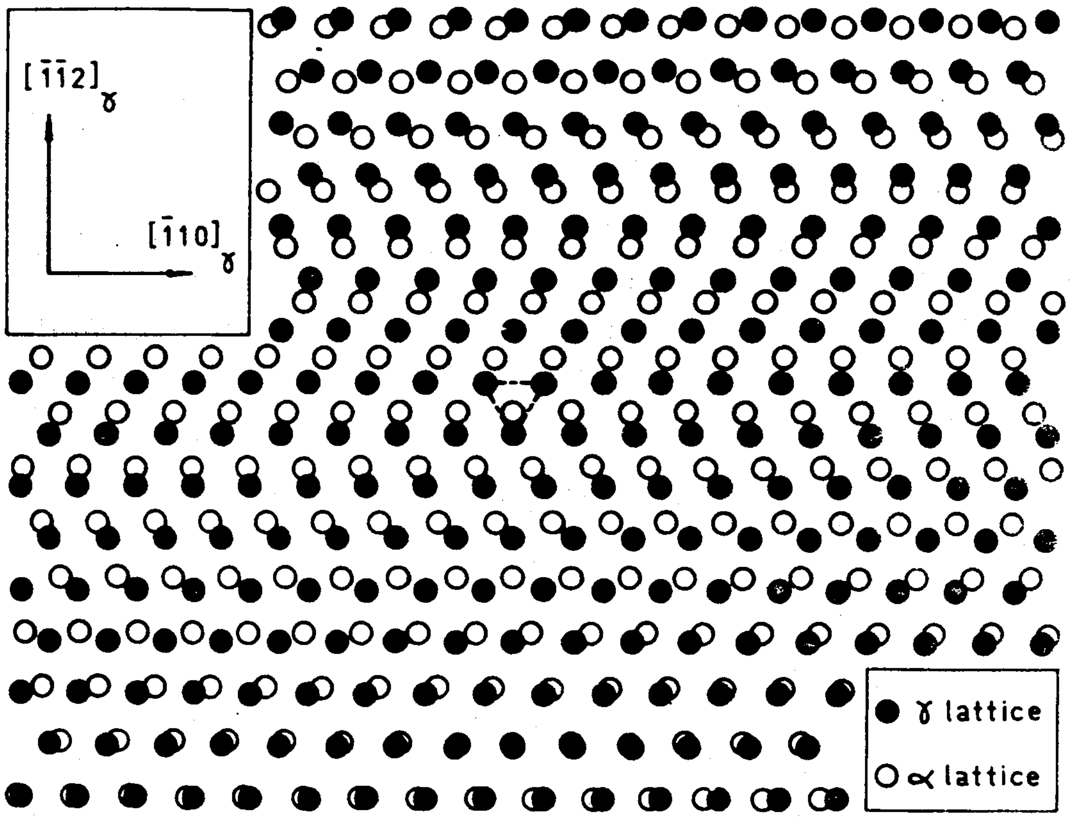
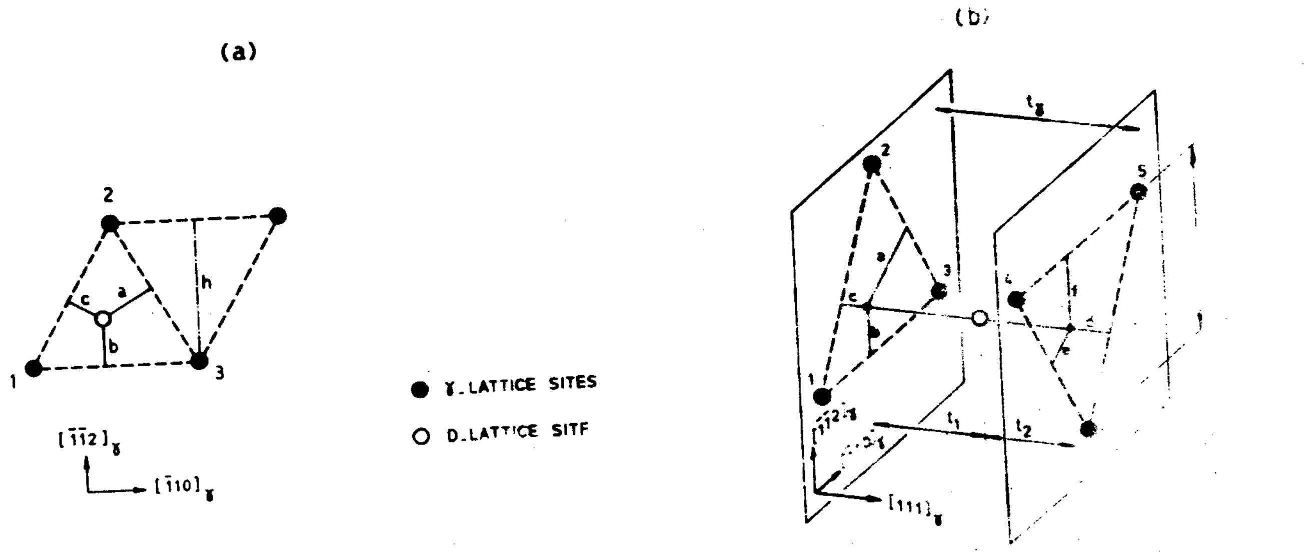


Fig. 1



$P_{I_{k_1}F_k} = \frac{a}{h}$ $P_{I_{k_2}F_k} = \frac{b}{h}$ $P_{I_{k_3}F_k} = \frac{c}{h}$

$P_{I_{k_1}F_k} = \frac{a}{h}\frac{t_2}{t_\gamma}$ $P_{I_{k_2}F_k} = \frac{b}{h}\frac{t_2}{t_\gamma}$ $P_{I_{k_3}F_k} = \frac{c}{h}\frac{t_2}{t_\gamma}$

$P_{I_{k_4}F_k} = \frac{d}{h}\frac{t_1}{t_\gamma}$ $P_{I_{k_5}F_k} = \frac{e}{h}\frac{t_1}{t_\gamma}$ $P_{I_{k_6}F_k} = \frac{f}{h}\frac{t_1}{t_\gamma}$

Fig 2

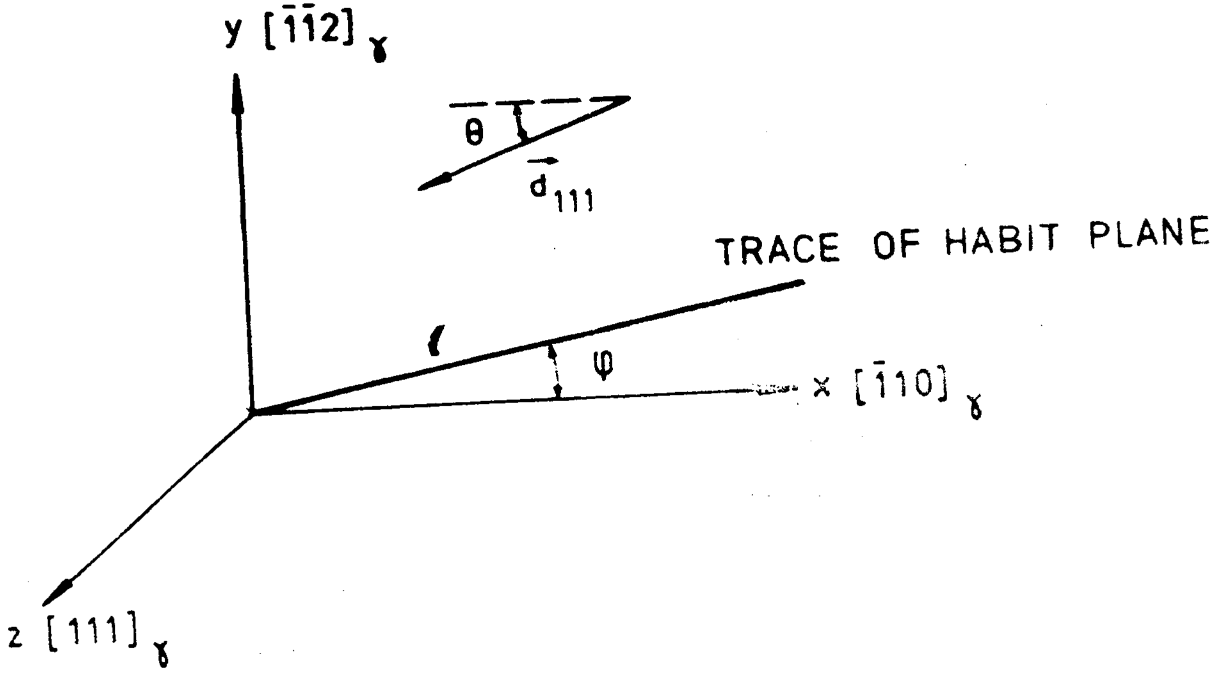

$y\ [\bar{1}\bar{1}2]_\gamma$
θ
$\vec{d}_{111}$
TRACE OF HABIT PLANE
ℓ
φ
$x\ [\bar{1}10]_\gamma$
$z\ [111]_\gamma$

Fig 3a

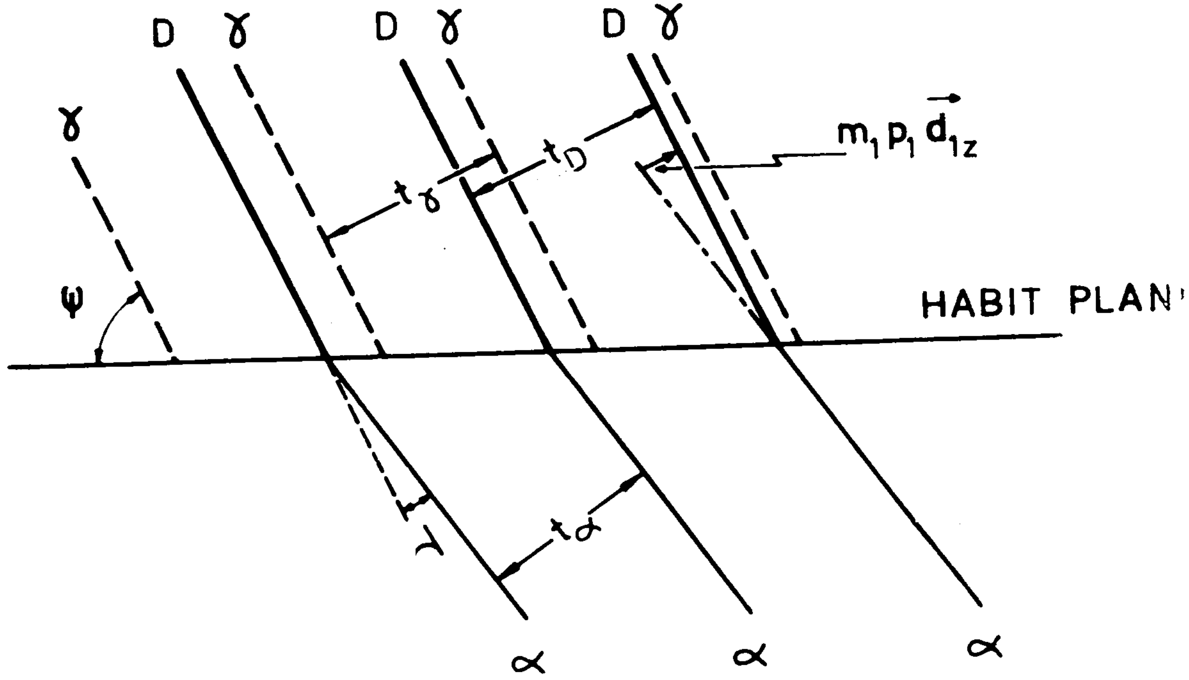

D
γ
D
γ
D
γ
γ
$m_1 p_1 \vec{d}_{1z}$
t_γ
t_D
ψ
HABIT PLAN'
λ
t_α
α
α
α

Fig. 3b

where D_i is the interphase boundary diffusion coefficient. Thus the probability distribution is realistic as long as

$$r \ll \frac{2}{\pi} \left(\frac{d\ D_i}{V} \right)^{1/2} \qquad (A2)$$

Taking for instance $dD_i \sim 10^{-14}$ cm^3 /sec and $V \sim 10^{-6}$ cm/sec, (A2) yields

$$r \ll 5 \times 10^{-5} \text{ cm}$$

which is a very small particle.

APPENDIX II

CALCULATION OF THE AVERAGE OF THE $p_{{}^I\vec{k}}$ DISTRIBUTION, IN THE CASE OF A HOMOGENEOUS DEFORMATION

Consider a probability distribution such that $\sum_{{}^I\vec{k}} p_{{}^I k {}^F k} = 1$, where all the ${}^I\vec{k}$ vectors in this sum denote positions in only one I plane for all the ${}^F\vec{k}$ vectors describing positions in one F plane. In view of the symmetry properties that characterize a crystalline solid, it may be stated that - under steady state growth conditions - the probability distribution will repeat itself with a certain periodicity. The period will depend on the lattice parameters of both the I and The F lattices and on the orientation relationship.

The average of $p_{{}^I k}$ over all the ${}^I\vec{k}$ vectors defining positions in the I plane considered is

$$\bar{p}_{{}^I k} = \overline{\sum_{{}^F\vec{k}} p_{{}^I k {}^F k}} = \frac{1}{N_I} \sum_{{}^I\vec{k}} \sum_{{}^F\vec{k}} p_{{}^I k {}^F k} = \frac{N_F}{N_I} \qquad \text{(A3)}$$

where N_F is the number of F lattice vectors in one period of the probability distribution in the plane, and N_I is the corresponding number of I lattice vectors. Unless the atom densities in both I and F planes being considered are equal, $N_F \neq N_I$. On the other hand, the N_F do not necessarily occupy the same area as the N_I atoms do. But, $N_F \equiv N_D$, where N_D is the number of D lattice points that do occupy the same area as the N_I ones. Then,

$$\bar{p}_{{}^I k} = \frac{N_D}{N_I} = \frac{\Delta_D}{\Delta_I} \qquad \text{(A4)}$$

where Δ_D and Δ_I are respectively the density of lattice points of the D and that of the I related planes.

APPENDIX III

CALCULATION OF THE PROBABILITY DISTRIBUTION FOR THE WIDMANSTATTEN FERRITE

The D planes associated through the correspondence (F C D) with the $(101)_\alpha$ planes, are parallel to the $(111)_\gamma$ planes.

For the data of Watson and McDougall (8), the trace of the habit plane in the $(111)_\gamma$ plane and the projection of the unit vector in the direction of the strain S_ε^{-1} are illustrated in fig. 3a. In fig. 3b, a view normal to that trace is sketched; the values of the pertinent angles and factors are given in Table VI. Then if x, y, z are the coordinates of an α lattice point referred to the system shown in fig. 3a,

$$
\begin{aligned}
S_\varepsilon^{-1}\, x &= x - m_1\,(y - x\,\mathrm{tg}\,\varphi)\,|d_{111}|\,\sin(\psi - \lambda)\,\cos\theta/0.9926 \\
S_\varepsilon^{-1}\, y &= y - m_1\,(y - x\,\mathrm{tg}\,\varphi)\,|d_{111}|\,\sin(\psi - \lambda)\,\sin\theta/0.9926 \qquad \text{(A5)} \\
S_\varepsilon^{-1}\, z &= z - m_1\,(y - x\,\mathrm{tg}\,\varphi)\,\sin(\psi - \lambda)\,|d_{1z}|/0.9926
\end{aligned}
$$

where $\vec{d}_{1z}$ is the component of the unit vector in the direction of the strain, normal to the $(111)_\gamma$ plane, and λ is the angle between the α and γ planes. $1 + m_1 p_1' d_1 = 0.9926$ for all the cases. The value of λ may be derived from (see fig. 3b)

$$\sin\lambda = m_1 \sin(\psi - \lambda)\,|d_{1z}|/0.9926 \qquad \text{(A6)}$$

The results are given in the first column of Table III.

The x and y coordinates that should be considered in equation (A5) are negligibly different from those that would obtain if the Kurdjumov-Sachs orientation relationship were strictly valid, provided $\lambda < 1°$, and thus the latter were taken in the calculation. Now, the component of displacement $S_\varepsilon^{-1} z$ does not change the x-y coordinates - relative to the sites of the $(111)_\gamma$ planes - of an α point already displaced by $S_\varepsilon^{-1} x$ and $S_\varepsilon^{-1} y$. Thus, the criterion described in the text for calculating the probability distribution (fig. 2a) may be applied without regard to the displacement in the z-direction (Tables III and IV). The distributions thus derived yield values of $p_{I_k} \neq 1$. Hence the possibility of independent atomic movements in the $[111]_\gamma$ direction has to be considered. The actual probabilities p_{I_k} should equal 1 since the system is conservative. Then using the same criterion as pictures in fig. 2b, it is easy to see , with the help of fig. 3b, that

$$p_{I_k} (2 t_\gamma - t_D) / t_\gamma = 1 \tag{A7}$$

But

$$t_D = t_\alpha \sin \psi / \sin (\psi - \lambda)$$

and hence

$$\sin (\psi - \lambda) = \frac{t_\alpha}{t_\gamma} \frac{\sin \psi}{2 - 1/p_{I_k}} \tag{A8}$$

permits to check the value of the angle λ (second column of Table III).