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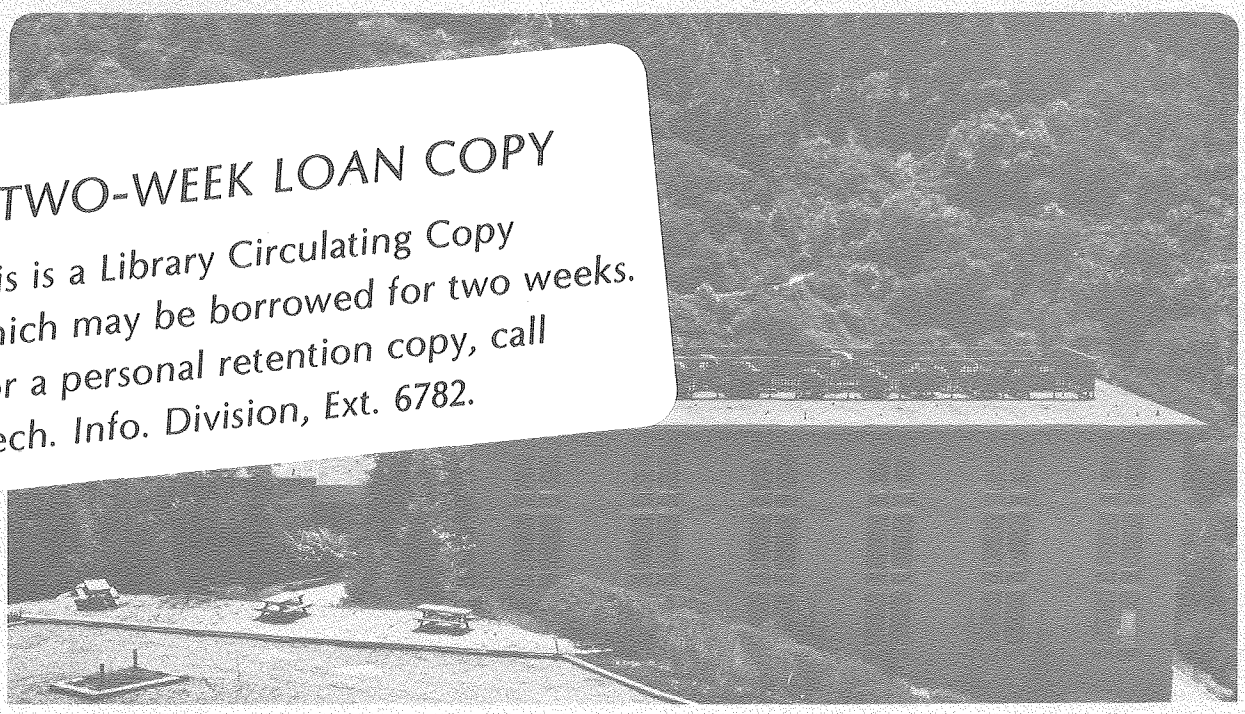

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The Role of the Invariant Line in the Search for an Optimum Interphase Boundary by O-Lattice Theory

In a recent publication[1], Plichta and Aaronson (PA) analysed the crystallography of the $\beta \longrightarrow \zeta$ massive transformation in Ag-Al alloys. One of the findings of this excellent study was that the Burgers orientation relationship (OR) (fig. 1) was preferred by almost all of the hcp ζ grains nucleated from the bcc β matrix. Most of the interphase boundaries were faceted and found to be partially coherent. The authors then used Bollmann's O-lattice theory[2] to determine the optimum interface and the corresponding orientation relationship in a manner similar to the classical analysis by Bollmann and Nissen.[3] The predictions of the O-lattice theory agreed very well with the experimental results. These predictions were based on the assumption that the optimum interface was partially coherent with two sets of dislocations accommodating the mismatch. The two Burgers vectors of these two sets of dislocations were selected from the ten shortest lattice translations of the hcp lattice. An energy parameter P was then calculated for the different interfaces corresponding to each pair of Burgers vectors. All the different combinations gave 45 possible interphase boundaries. The boundary with the smallest energy parameter P was found to be an interface described directly by the Burgers OR (fig. 1). Even though there was good agreement with the experiments, PA added a further refinement to their calculations by testing the stability of this minimum under small rotations. Without these additional rotations, the two lattices, hcp and bcc, were related by a transformation matrix $\hat{A}$ whose form was

determined by their choice of two pseudo-primitive unit cells. While this choice did not eliminate the need for an additional shuffle to produce the correct atomic positions, its advantage over the more conventional choice of orthogonal unit cells[5] was that it created one lattice from the other in the exact Burgers OR (fig. 1) as experimentally observed. (Orthogonal unit cells lead to the Pitsch/Schrader OR[6] shown in fig. 2). Thus the rotations around three mutually orthogonal axes were designed to determine whether the Burgers orientation relationship did indeed provide the lowest energy boundary. With the aid of a computer program, the energy parameter P was calculated as a function of these rotations for each of the 45 possible boundaries. Again it was found that the same interface had the lowest energy but, interestingly, it was noted that this boundary had its absolute minimum at an OR rotated about 0.05^{o} around $[0001]$ away from the exact Burgers OR. In view of this small deviation, the authors therefore concluded correctly that "the Burgers OR appears to follow directly from minimization of the interphase boundary energy". They also pointed out that an OR is established during nucleation rather than during growth, all interfaces being fully coherent during nucleation. However, they then stated that "the smaller the P_{ij} value of an interface, the less the strain energy required to achieve full coherency", implying that the optimum boundary is the same for coherent and incoherent precipitates, a fact which does not necessarily follow. The purpose of the present communication is threefold:

-to demonstrate that the interphase boundary determined by PA can be shown analytically to have the lowest energy parameter P of all possible O-lattice boundaries.

-to explain the significance of the calculated 0.05^{o} rotation around [0001] and its relationship to the more general principle of an invariant line.

-to show that the optimum interphase boundaries are generally quite different for coherent and semicoherent precipitates having the same OR with the matrix.

The derivation of the O-lattice is based on the generalization of the principle of coincidence site lattices. The idea can be summarized shortly as follows. Two lattices may be related by a linear homogeneous transformation $\hat{A}$ which takes any point $\underset{\sim}{x}_1$ in lattice 1 to a new position $\underset{\sim}{x}_2$ in lattice 2:

$$\underset{\sim}{x}_2 = \hat{A}\underset{\sim}{x}_1.$$

The new point $\underset{\sim}{x}_2$ in lattice 2 is an O-lattice point $\underset{\sim}{x}^{o}$ if it is separated from its original position $\underset{\sim}{x}_1$ by a translation vector $\underset{\sim}{b}$ of lattice 1.

$$\underset{\sim}{x}_2 = \underset{\sim}{x}^{o} = \underset{\sim}{x}_1 + \underset{\sim}{b}$$

$$\underset{\sim}{x}^{o} = \hat{A}^{-1}\underset{\sim}{x}^{o} + \underset{\sim}{b}$$

$$(\hat{I} - \hat{A}^{-1})\underset{\sim}{x}^{o} = \underset{\sim}{b} \qquad (1)$$

This is the well-known basic equation of O-lattice theory.[2] If $\det|\hat{I} - \hat{A}^{-1}| \neq 0$, the equation can be solved for $\underset{\sim}{x}^{o}$:

$$\underset{\sim}{x}^{o} = (\hat{I} - \hat{A}^{-1})^{-1}\underset{\sim}{b} \qquad (2)$$

Every one of the translation vectors $\underset{\sim}{b}_i$ of lattice 1 has a corresponding O-lattice vector $\underset{\sim}{x}_i$. Every two O-lattice vectors define a possible interface

between lattice 1 and lattice 2. For n different translation vectors $\underset{\sim}{b}_i$ and hence n different O-lattice vectors $\underset{\sim}{x}_i^o$ there are $N = \sum_{i=1}^{n} (n-i)$ possible boundaries; PA chose $n = 10$ translation vectors and investigated $N = 45$ boundaries. The energy of each interface is proportional to the square of the strains and has been written by Bollmann and Nissen[3] as

$$P = \frac{(\underset{\sim}{b}_1)^2}{d_1^2} + \frac{(\underset{\sim}{b}_2)^2}{d_2^2} \qquad (3)$$

where $\underset{\sim}{b}_1$ and $\underset{\sim}{b}_2$ are two of the translation vectors $\underset{\sim}{b}_i$ and d_1 and d_2 are the spacings of the corresponding two sets of dislocation lines in the interface. The spacing d_1 is related to the O-lattice vectors by

$$d_1^2 = \frac{1}{(\underset{\sim}{x}_2^o)^2} (\underset{\sim}{x}_1^o \times \underset{\sim}{x}_2^o)^2$$

and d_2^2 is obtained by an interchange of indices. The energy parameter can thus be rewritten as

$$P = \frac{(\underset{\sim}{b}_1)^2(\underset{\sim}{x}_2^o)^2 + (\underset{\sim}{b}_2)^2(\underset{\sim}{x}_1^o)^2}{(\underset{\sim}{x}_1^o \times \underset{\sim}{x}_2^o)^2} \qquad (4)$$

Apparently P is a function of the magnitudes of the $\underset{\sim}{b}_i$ and $\underset{\sim}{x}_i^o$, of the angle between the $\underset{\sim}{x}_i$ and, implicitly, of the OR. It is helpful to examine the behavior of P as a function of each of these parameters separately.

For a given angle between $\underset{\sim}{x}_1^o$ and $\underset{\sim}{x}_2^o$ and a given OR, the energy parameter P is actually independent of the magnitudes of the translation vectors $\underset{\sim}{b}_i$. Since the transformation from the $\underset{\sim}{b}$ lattice to the O-lattice, $(I - A^{-1})^{-1}$, is linear (equ. 2), an n- and m-fold increase in $\underset{\sim}{b}_1$ and $\underset{\sim}{b}_2$ will cause an n- and m-fold increase in $\underset{\sim}{x}_1^o$ and $\underset{\sim}{x}_2^o$. Using this in equ. 4

shows that the factors m^2n^2 cancel and that P is independent of the magnitudes of the Burgers vectors. According to this result, a boundary containing a network of dislocations $\underset{\sim}{b}_i$ with spacings d_i has the same energy as a boundary with half the number of dislocation lines (spacing $2d_i$) and twice the Burgers vector, $2\underset{\sim}{b}_i$. This is, of course, a shortcoming of the energy parameter since a dependence of the magnitude of the $\underset{\sim}{b}_i$ must exist. PA acknowledged this fact indirectly when they listed their Burgers vectors in order of increasing magnitude (normalized line energy).

The dependence of P on the angle between $\underset{\sim}{x}_1^o$ and $\underset{\sim}{x}_2^o$ is clear from the denominator of equ. 4, $(\underset{\sim}{x}_1^o \times \underset{\sim}{x}_2^o)^2$. P is a minimum if

$$(\underset{\sim}{x}_1^o \times \underset{\sim}{x}_2^o)^2 = (\underset{\sim}{x}_1^o)^2(\underset{\sim}{x}_2^o)^2 - (\underset{\sim}{x}_1^o \cdot \underset{\sim}{x}_2^o)^2$$

is a maximum. This is the case when $\underset{\sim}{x}_1^o$ is perpendicular to $\underset{\sim}{x}_2^o$. For the transformation strains of the $\beta - \zeta$ massive transformation in the Burgers OR, as used in the work of PA, most $\underset{\sim}{x}_1^o$ and $\underset{\sim}{x}_2^o$ are perpendicular when $\underset{\sim}{b}_1$ and $\underset{\sim}{b}_2$ are perpendicular. Generally this correlation between the O-net and the b-net only holds if the $\underset{\sim}{b}_i$ lie in the plane defined by the corresponding $\underset{\sim}{x}_i^o$. This condition defines an "eigenplane" of the transformation, i.e. a plane which remains parallel during the transformation. Hence the minimization of P requires that the two Burgers vectors $\underset{\sim}{b}_1$ and $\underset{\sim}{b}_2$ are approximately normal (exactly normal if they lie in an eigenplane of the transformation). This is the case for the c-dislocation with one of the a-dislocations in an hcp lattice. Of the three a-dislocations only one defines an eigenplane with the c-direction. With a 0.31% expansion in the a-direction and a 0.04% contraction in the c-direction (for Ag-Al), the strain in this plane is small and hence the O-points are widely spaced. This plane therefore minimizes the energy

parameter P with respect to the choice of the $\underset{\sim}{b}$-vectors at a given OR, in perfect agreement with the computations of PA for the exact Burgers OR.

In the second step of their analysis, PA sought a further reduction of the energy parameter by relaxing the condition that the exact Burgers OR be followed. They changed the OR by superimposing small rigid body rotations upon the original transformation. For small rotation angles, a rotation around an arbitrary axis can be approximated by three separate rotations around orthogonal axes. The energy parameter P of the minimum energy boundary can be plotted as a function of these three separate rotations with the aid of a computer program. Using this approach, PA found an absolute minimum of P for a 0.05^{o} rotation around $[0001]$.

This may also be readily understood by returning to equ. (3). Regarding the terms $\frac{|\underset{\sim}{b}_i|}{d_i}$ as continuous strains in the directions of the O-lattice vectors, it can be shown that under certain conditions one of these strains can be reduced to zero by a rigid body rotation. This can be visualized as the spacing of the dislocation lines d_i going to infinity, or perfect atomic fit in that direction. This direction is an invariant line of the transformation. In the case treated by PA, the rotation that produces the invariant line does not affect the other strain. Thus the dislocation spacing

in the direction of the rotation axis [0001] remains constant. The rotation which produces an invariant line therefore defines the OR for which the boundary energy P has an absolute minimum. The general case requires a more refined argument which will not be discussed here. It is easy to calculate the angle of rotation θ necessary to produce an invariant line. As shown in more detail in a separate publication,[7] this angle is given by

$$\theta = \cos^{-1}\left(\frac{1 + ab}{a + b}\right) - 5.264^{o}$$

where a and b are the orthogonal components of the pure deformation creating one lattice from the other in the plane of rotation; 5.264^{o} is the difference between the Pitsch/Schrader OR used in the derivation of θ[7] and the Burgers OR used by PA. For the case of the $\beta \longrightarrow \zeta$ transformation of PA, the orthogonal deformations are

$$a = 0.869 \qquad b = 1.064$$

and hence θ is calculated as

$$\theta = 0.079^{o} \quad .$$

This agrees well with the value of approximately 0.05^{o} calculated by computer program in the study of PA. While the present approach adds little to the accuracy of the OR, it is simpler than the computerized approach and brings to light another property of the lowest energy boundary. Due to the invariant line, the O-lattice becomes a line lattice as originally pointed out by Bollmann.[2] An invariant line is defined as that vector $\underset{\sim}{x}$ which remains unstretched and unrotated by

the transformation $\hat{A}$.

$$\hat{A}\underset{\sim}{x} = \underset{\sim}{x} \quad \text{or} \quad \underset{\sim}{x} = \hat{A}^{-1}\underset{\sim}{x}$$

Hence $(\hat{I} - \hat{A}^{-1})\underset{\sim}{x} = 0$ which means that

$$\det|\hat{I} - \hat{A}^{-1}| = 0$$

and $(\hat{I} - \hat{A}^{-1})$ has no inverse. Eq. (1) can therefore not be solved for $\underset{\sim}{x}^{o}$. In the vicinity of the critical rotation θ, however, the inverse of $(\hat{I} - \hat{A}^{-1})$ does exist and (1) can be solved by (2) as in the calculations of PA.

Relationship of the optimum O-lattice to interfaces of a coherent nucleus. Based on the analysis of PA and the arguments presented in the preceding paragraphs, the optimum interface contains a single set of dislocations parallel to the invariant line and requires that the OR be rotated slightly away from the ideal Burgers OR. PA concluded that this interface must also be an optimum interface for a coherent nucleus; according to nucleation theory, a slight advantage in the coherency strain energy leads to a great increase in nucleation rate for nuclei with the calculated OR and interface. While the latter part of this argument is correct, the former part needs closer examination. Assume that the OR is the same for a coherent and a semicoherent precipitate. Then lattices 1 and 2 are related by a corresponding transformation matrix $\hat{A}$. To minimize coherency stresses, the interfaces of a coherent nucleus with the matrix must be planes of minimum distortion. Because of the continuous nature of $\hat{A}$, the coherent interfaces are completely independent of the periodicity of the lattice. This is

different for semicoherent interfaces which are governed by the requirement that in the interface the continuous strains are periodically eliminated. Wherever the continuous strains amount to a perfect lattice translation, the match is perfect and a point of no strain or an O-lattice point, is established. Hence semicoherent interfaces are dominated by both, minimum strain and lattice periodicity. In the interface, the continuous strains always lie in the direction of the Burgers vectors of the misfit dislocations. However, in general, the Burgers vectors do not have to lie in the interface[2], i.e. $\underset{\sim}{b}_1 \times \underset{\sim}{b}_2$ defines a plane which is usually not parallel to $\underset{\sim}{x}_1^o \times \underset{\sim}{x}_2^o$.

Hence semicoherent boundaries are not simply restricted to planes which suffer the smallest distortion during the transformation $\hat{A}$.

These considerations hold for any OR given by the matrix $\hat{A}$. In the particular case of an OR producing an invariant line, both optimum boundaries, coherent and semicoherent should contain that line. This is because the invariant line fulfills the conditions for both boundaries; minimum strain and no change in direction. Hence the two boundary planes will intersect in the invariant line.

Summary and conclusions.

Using the example of a recent study by Plichta and Aaronson (PA)[1] their results on the optimum O-lattice interface and corresponding orientation relationship (OR) were generalized. In particular, it was shown that

-for any OR, the minimum energy interface is based on dislocations in a (nearly) orthogonal network ($\underset{\sim}{x}_1^o \cdot \underset{\sim}{x}_2^o = \min$).

-an absolute minimum in interface energy occurs at an OR which provides an invariant line.

-the optimum boundary contains a single set of dislocations parallel to the invariant line.

-the OR, determined during nucleation, depends on the minimum energy coherent interfaces which are generally different from their semi-coherent counterparts.

-if an invariant line exists, it is the line of intersection of the optimum coherent and semicoherent interfaces.

The results are in full agreement with those of PA. A more complete account of the general significance of the invariant line in phase transformations is in preparation[7].

Acknowledgements

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Figure Captions

Fig. 1. Burgers orientation relationship between bcc lattice (3-index poles) and hcp lattice (4-index poles). Coincident poles are marked.

Fig. 2. Pitsch/Schrader orientation relationship, rotated 5.26^{o} from the Burgers relationship in Fig. 1. (Note its higher symmetry.)

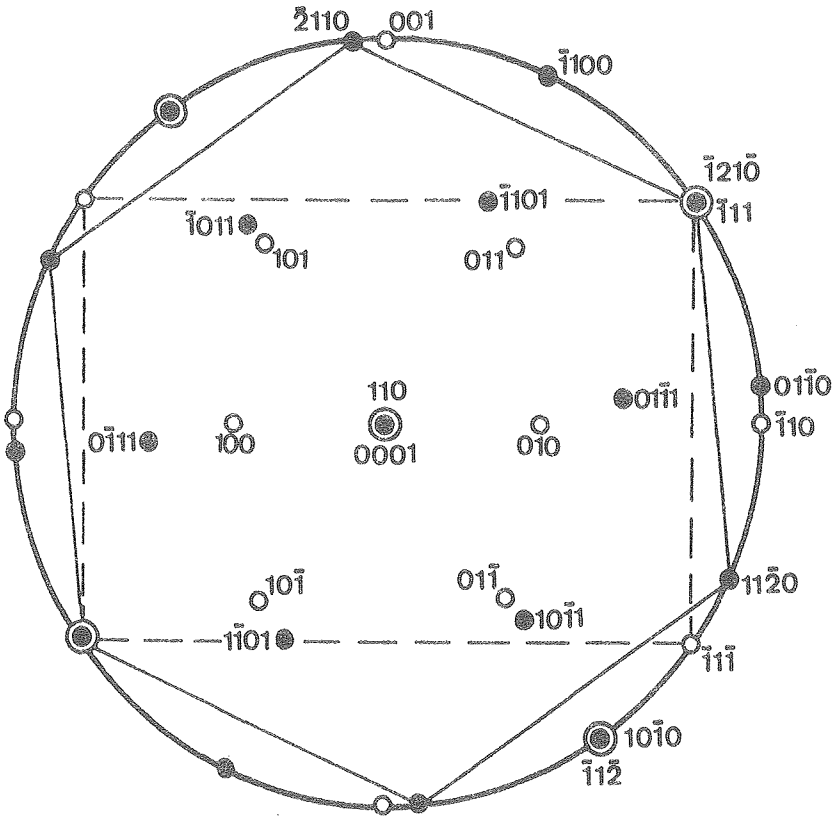
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Fig. 1

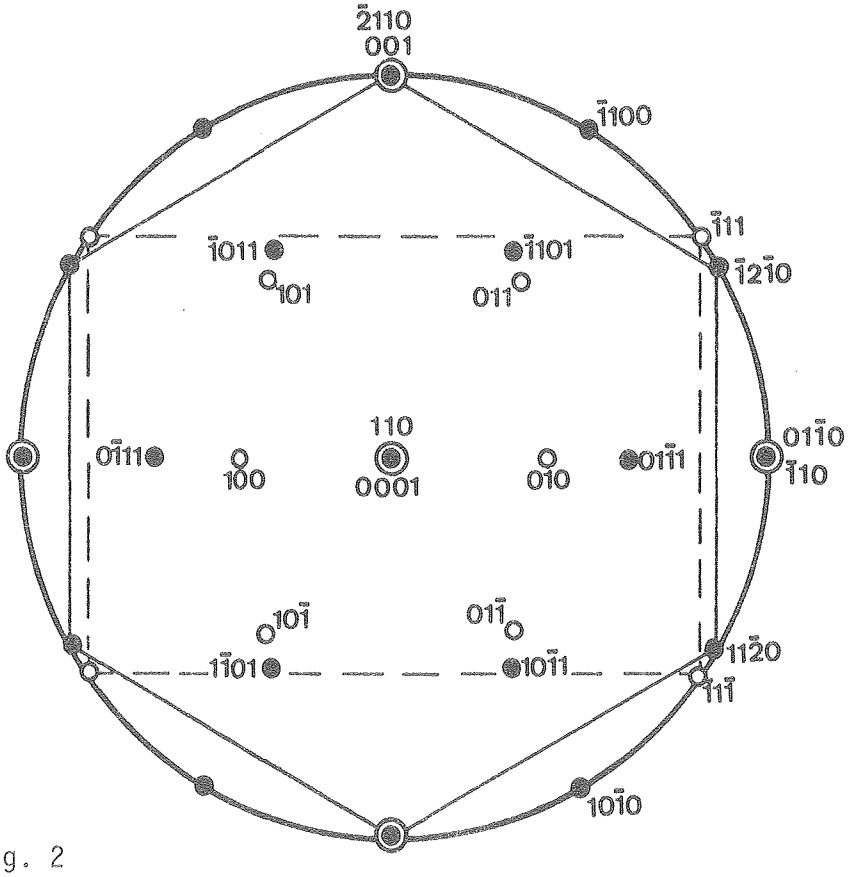
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Fig. 2