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Review

Problems in the Calculation of Transformation Texture in Steels

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The solid-state decomposition of austenite can lead to a non-random distribution of product crystals. Methods of the quantitative characterisation of this texture are extremely advanced, and there is a deep understanding of the relationship between the texture and macroscopic properties. There remain, however, important barriers to the complete calculation of texture, some of which have not been documented in the published literature. It is the purpose of this review to focus on the difficulties in order to set the scene for further progress. The advent of electron back scatter diffraction has led to an explosion of papers on microscopic aspects of crystal orientations; some of the issues relating to this technique are also described.

KEY WORDS: transformation texture; crystallography; steel; martensite; bainite.

1. Introduction

Crystallographic texture occurs when the distribution of crystal orientations is not random relative to a macroscopic frame of reference. An understanding of the subject can help relate single-crystal properties to those of aggregates of crystals[1,2] and the design of grain boundaries.[3–8] The distribution of grain orientations can become biased as the individual crystals rotate in compliance with the imposed deformation; thus in hexagonal close-packed zirconium, the basal planes of the grains tend to align with the rolling plane during the production of sheet.[9] Selective phenomena during recovery, recrystallisation and grain growth can change the character of the final texture.[10,11] Epitaxy during deposition obviously can lead to textures in coatings[12,13] as does heat-treatment in an electrical or magnetic field.[14,15] The goal of this paper is, however, to deal with only one of these many mechanisms, the texture that develops when a solid-state phase transformation occurs in steel under the influence of external forces. As will be seen later, there are parts of the subject which are particularly amenable to calculation and others which are not.

2. Single Crystals, Imperfections and EBSD

Crystallography had little influence on the development of practical materials until well into the last century.[16] The classification of crystals according to their equilibrium shape and an understanding of symmetry laid the foundations of the subject, with more progress when the interactions between waves and crystals were expressed in the form of the Bragg equation. The allotropic forms of iron were thus resolved using X-rays in 1921,[17,18] and proof soon emerged that β-iron does not exist.[19]

It is important to remind ourselves that the Bragg law is formulated for a perfect crystal which is large. The size is important in order to avoid diffracted intensity around the exact Bragg angle. Perfection here implies long-range periodicity; defects such as dislocations and disordered solutions disrupt the periodicity; furthermore, high-entropy defects such as vacancies can exist at equilibrium so it may be impossible to produce sizeable crystals which present sharp diffraction peaks. It is only possible to approximate perfection in small crystals[20] and even there, the surface of the crystals is likely to be reconstructed.[21,22] Modern materials rely on imperfections for their properties,[23] and these will cause the angular broadening of diffracted intensity.[24]

Electron backscatter diffraction (EBSD) is now common in the study of microtexture. The resulting information however, has to be interpreted with caution with respect to both the spatial and angular resolution, particularly when interpreting orientation relationships and grain boundaries.

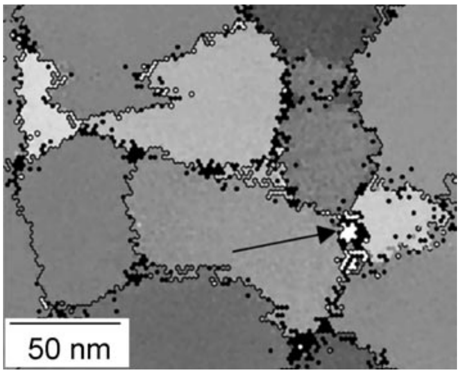

Fig. 1. Grain structure in a platinum film, resolved using EBSD. With kind permission from Springer Science+Business Media from "the use of electron backscatter diffraction for the investigation of nano crystalline materials and the move towards orientation imaging in the TEM", *Microchimica Acta*, **147** (2004), 157, Fig. 4(b).

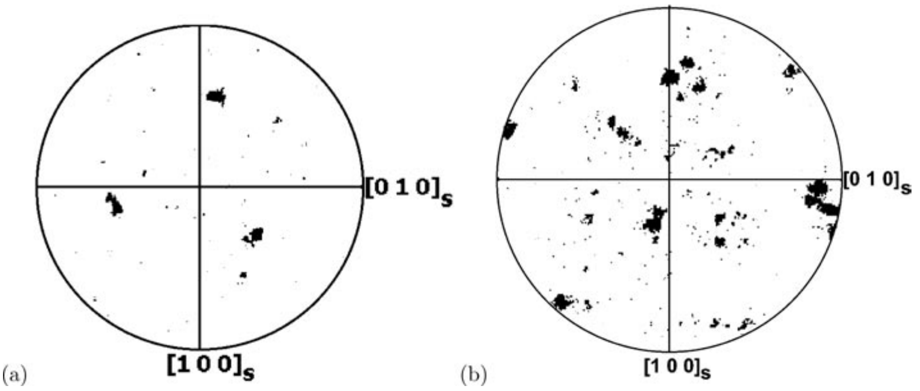

Fig. 2. Pole figures from a single crystal of austenite which is partially transformed into bainite.[27] (a) $1\,0\,0_\gamma$ pole figures, (b) Corresponding $1\,0\,0_\alpha$ pole figure.

Consider first the spatial resolution. Using a step size of 2–4 nm might suggest a resolution of that order, but **Fig. 1** illustrates the difficulties. The boundaries in this image appear convoluted whereas they are not in reality. The grain marked with an arrow is suggested to have a size of about 8 nm[24] but it is questionable whether this is a real grain or an artefact given the size of the surrounding black regions which are crystallographically unresolved pixels. The grain boundaries themselves appear ragged, with a roughness which is comparable to the suggested 8 nm grain. Such roughness is not likely to be real since and thin film deposition does not normally lead to a bimodal distribution in grain size.

Consider now the problem of angular resolution when dealing with steels. The influence of imperfections in causing a spread in orientation well beyond the stated angular resolution of the EBSD instrument is illustrated in **Fig. 2**(a). Instrumental resolution should be of the order of 0.5° but the illustrated spread in the orientation of the single grain of austenite is closer to 10°. There will then be a corresponding spread in the orientations of bainite, as illustrated in Fig. 2(b), even if there is a strictly fixed orientation relationship between the parent (γ) and product (α) phases. Products which form by displacive transformations will contain excess dislocations leading to a spread in diffracted intensity. Furthermore, the contribution to the spread from different crystals of bainite or martensite will not be identical given the nonuniform distribution of dislocations, plastic accommodation and the fact that the stress state of the austenite changes as more plates of martensite form.[25] There are many publications in the literature which suggest that there is a spread in the γ/α orientation relationship rather than one established by the crystallography of the phases. It is then reasonable to question whether there is a true spread in orientation relationship or one which is caused by a neglect of the fact that the austenite is not a perfect crystal. The measurements implying spread have in some cases been deduced from observations on meteorites, which cool incredibly slowly as they evolve to their final structure. In these circumstances, there must be orientation changes due to the recovery of defect structures.

To summarise, it is not yet proven that EBSD measurements which indicate a spread in diffracted intensity are due to the variation in γ/α orientation relationships. Texture calculations can proceed on the basis of well-defined parent-product orientation relationships. The focus should be on understanding and predicting the expected spread in the orientation of austenite due to plastic accommodation effects associated with displacive transformation mechanisms.[26]

3. Calculation of Texture due to Displacive Transformations

Displacive transformations are particularly simple because the product phase grows by a synchronised movement of the atoms in the parent phase, leading to a well-defined orientation relationship. Furthermore, this orientation relation is dependent only on the parent crystal in which the transformation occurs because the displacive transformation is confined within the grain in which it occurs, **Fig. 3**. The crystallographic texture can therefore be estimated from a knowledge of the orientations of the parent crystals and their orientation relationship with the product phase.[28] The theory for displacive transformations[29–34] is far more developed than their reconstructive counterparts. It is possible for each plate of martensite, bainite or Widmanstätten ferrite to uniquely define the indices of its habit plane, the deformation caused by transformation and the orientation relationship using the phenomenological theory of martensite crystallography which mathematically relates these three parameters.

The full theory[29–31] is beyond the scope of this paper; detailed descriptions and reviews can be found elsewhere.[32,34–36] The theory predicts that the crystallographic indices representing the orientation relationship and habit plane are in general irrational; that means that the indices cannot be expressed by the division of integers. This necessarily means that there will be 24 variants of the transformation product per austenite grain. As a corollary, simplified descriptions of the orientation relation in terms of Kurdjumov–Sachs[37] and Nishiyama–Wasserman[38,39] are imprecise in detail; thus, the latter orientation would lead to only twelve variants. As far as the author is aware, there has never been experimental confirmation that only twelve variants of martensite can form in a given austenite grain.

If all 24 variants are allowed to form in each austenite grain, then the transformation texture becomes essentially random for any sizeable sample of material. However, circumstances may force variant selection, *i.e.*, where certain

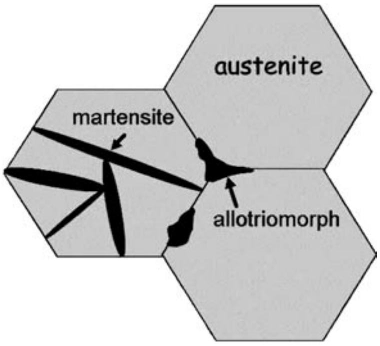

Fig. 3. An illustration of the fact that martensite, bainite and Widmanstätten ferrite, all grow in the form of 'plates' which do not cross austenite grain boundaries because it is not possible to sustain a disciplined motion of atoms through a change in crystallographic orientation. In contrast, the growth of allotriomorphic ferrite or pearlite occurs by a reconstructive mechanism involving long-range diffusion so that the growing particle is not confined to the grain in which it nucleates.

crystals which are more compliant to an external influence, such as a macroscopic stress or magnetic force, tend to form in preference. Magnetic fields are interesting but impractical, so it is much more interesting to examine the effect of stress.

Displacive transformations are typified both by a change in crystal structure and a large deformation. The strain due to martensitic transformation occurs on the habit plane (unit normal **p**) in a displacement direction (unit vector **d**). Unlike simple shear, **d** will not lie precisely in the habit plane because the volume change of transformation is directed normal to the habit plane. The dominating strain is the shear parallel to the habit plane at about 0.26. The total deformation is expressed as a 3×3 matrix **P**:

$$(\gamma \ \mathrm{P} \ \gamma) = \mathrm{I} + m[\gamma; \mathbf{d}](\mathbf{p}; \gamma^*) \ \ldots\ldots\ldots\ldots\ldots\ldots(1)$$

where m is the magnitude of the shape deformation and γ and γ^* represent the real and reciprocal bases of the austenite. The matrix **P** thus completely defines the deformation system, and there will in general be 24 different variants.

It is most important to realise that the Bain strain (**B**), rigid body rotation (**R**), and the shape deformation (**P**) are all mathematically related through the phenomenological theory of martensite:

$$\mathbf{P} = \mathbf{BR}(\mathbf{P}')^{-1} \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

where **P**′ is a shear whose macroscopic consequence is cancelled by the lattice-invariant deformation. Equation (2) emphasises that the orientation relationship and shape deformation are mathematically related. It is not rigorous to assign an orientation and then use independent data for the shape deformation, as is sometimes done.[40–42] Similarly, the use of shears which are consistent with an assumed orientation relationship but not with the habit plane[43] contradict the need for a self-consistent mathematical set.

It is the interaction of the applied stress with **P** which determines variant selection. The interaction energy which provides the mechanical driving force for transformation is given by[44]:

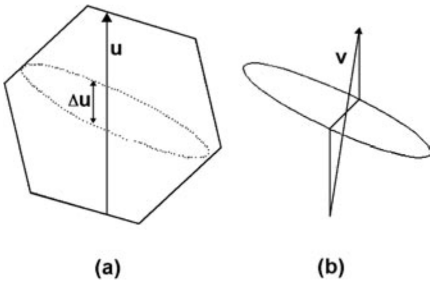

Fig. 4. The deformation of an initial vector **u** by the formation of bainite. (a) An austenite grain prior to transformation, with the ultimate location of a plate of bainite marked. (b) Following displacive transformation.[27]

$$U = \sigma_N \zeta + \tau s \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

where σ_N is the stress component normal to the habit plane, τ is the shear stress resolved on the habit plane in the direction of shear and ζ and s are the respective normal and shear strains associated with transformation. The energy U can be used as a rigorous variant selection criterion when the role of any plastic strain is unimportant.[27] Note that it is **P** which is the macroscopic deformation due to transformation and which must therefore be used to calculate the interaction energy (variant selection) rather than, for example, the Bain strain which has sometimes been applied, *e.g.*[45]

4.1. Transformation Plasticity

With displacive transformations it is possible to calculate the macroscopic plastic-strains as a function of texture; they can also be used to characterise the texture because they are in general anisotropic.[27,46,47] An arbitrary vector **u** traversing a grain of austenite prior to transformation (**Fig. 4**(a)) makes an intercept Δ**u** with a domain of austenite that eventually transforms, after which it becomes a new vector **v** given by:

$$\mathbf{v} = \mathbf{P}\Delta\mathbf{u} + (\mathbf{u} - \Delta\mathbf{u}) \ \ldots\ldots\ldots\ldots\ldots\ldots(4)$$

When many plates form in many austenite grains, **u** traverses a polycrystalline sample of austenite so this equation is generalised as follows[27]:

$$\mathbf{v} = \sum_{k=1}^{n} \sum_{j=1}^{24} \mathbf{P}_j^k \Delta\mathbf{u}_j^k + \left(\mathbf{u} - \sum_{k=1}^{n} \sum_{j=1}^{24} \Delta\mathbf{u}_j^k \right) \ldots\ldots(5)$$

where $j = 1 \ldots 24$ represents the 24 crystallographic variants possible in each austenite grain, and $k = 1 \ldots n$ represents the n austenite grains traversed by the vector **u**. In this scenario of a large number of bainite plates, the intercepts $\Delta\mathbf{u}_j^k$ can be approximated by $f_j^k\mathbf{u}$ where f_j^k is the fraction of sample transformed by variant j in austenite grain k.

The deformation caused by a particular plate j in austenite grain k, *i.e.*, $(\gamma_k \mathrm{P}_j \gamma_k) \equiv \mathbf{P}_j^k$. The remaining 23 such matrices for grain 1 of austenite can be deduced from this using symmetry operations. They can then be expressed in the reference frame of the sample using a similarity transformation as follows:

$$(\mathrm{S}\ \mathrm{P}_j^k\ \mathrm{S}) = (\mathrm{S}\ \mathrm{R}\ \gamma_k)(\gamma_k\ \mathrm{P}_j\ \gamma_k)(\gamma_k\ \mathrm{R}\ \mathrm{S}) \ \ldots\ldots\ldots(6)$$

where $(\mathrm{S}\ \mathrm{R}\ \gamma_k)$ is the rotation matrix relating the basis vectors of the kth austenite grain to the sample axes, and

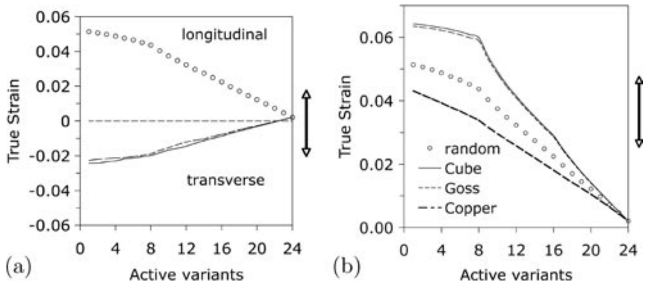

Fig. 5. These diagrams show the plastic strain that develops in a sample of 500 austenite grains placed under tension along the longitudinal axis. The differences in the orthogonal strains correlate with the intensity of transformation texture, assuming that each variant that forms contributes equally to the fraction of transformation. (a) Strains developed due to transformation along the $[1\,0\,0]_S$ direction (labelled longitudinal, along the stress axis), and the transverse directions $[0\,1\,0]_S$ and $[0\,0\,1]_S$. (b) Tensile stress, but transformation beginning from a variety of starting austenite textures and illustrating only the longitudinal stress.[27]

(γ_k R S) is the inverse of that rotation matrix. In this way, the calculation described in Eq. (4) can be conducted in the sample frame of reference.

Some calculations illustrating the anisotropy of strains as a function of the number of crystallographic variants of martensite allowed are illustrated in **Fig. 5**(a) for uniaxial tension when transformation occurs from a randomly oriented set of austenite grains. That displacive transformations produce highly anisotropic strains when variant selection is significant has been demonstrated experimentally.[46–48]

Figure 5(b) shows that transformation texture is absent when 24 variants form in each austenite grain, for typical intensities of texture in the austenite; the only strain visible in these circumstances is the an averaged isotropic volume expansion. The strength of the transformation texture increases as the number of variants per austenite grain decreases.

An important outcome of the fact that transformation strains can be calculated using the crystallographic set of martensite is that such strains can be exploited as an alternative or supplemental method of assessing texture. It is also possible to estimate aspects of the 'microstructure' since the orientation of the habit plane of each plate is an outcome of the analysis.

4. Description of the Polycrystalline State

We have seen that for displacive transformations, the habit plane, orientation relationship and shape deformation are mathematically linked. The habit cannot be changed independently of the other two characteristics. This is not generally true for bicrystals, where the interface plane can be changed independently of the crystal orientation. In this section we consider the complexity that arises when we abandon the restrictions imposed by the displacive transformation mechanism and permit greater degrees of freedom.

The manipulation of grain boundaries in order to achieve specific properties was known originally as 'grain boundary design'[3] and later as 'grain boundary engineering'.[4–8] Since the field began, the focus has been on the correlation of the orientations of the crystals against properties, not specifically the structure of grain boundaries. Whereas it may be reasonable to associate the character of boundaries with the orientation relationship between the grains it connects,[49] this relationship is not straightforward.[34,35,50] The reason why the focus is not on grain boundaries *per se* can be understood when the variables required to describe the polycrystalline state are enumerated.

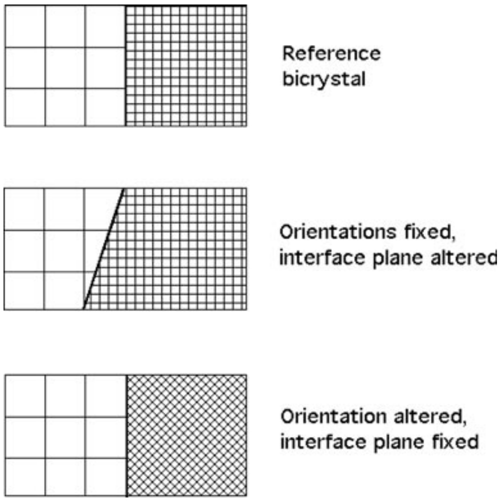

Fig. 6. An illustration of the fact that the orientation relationship between crystals can be independently varied without altering the plane of the interface and *vice-versa*. If the two crystals belong to same crystal class (of which there are seven) then the orientation relation can be described by an axis and an angle of rotation about that axis. The interface plane is specified by an axis normal to the plane. Since each axis can be written as a unit vector we need specify only two of its components. Thus, the total degrees of freedom required to specify the bicrystal is five.

The formal description of a polycrystal is complicated because additional variables are required when compared with the single crystal. There are at least five degrees of freedom needed to specify a bicrystal in which the two components are joined at a single interface (**Fig. 6**); three for the relative orientation of the two crystals and two in order to represent the normal to the interface plane. Additional degrees of freedom may be needed if the interfacial energy can be reduced by a translation of the two lattices by a fraction of the repeat distance in a direction parallel to the interface,[51] although it is not clear how such a translation can be accommodated in a three-dimensional polycrystal where the surrounding material provides a constraint.

The problem is made severe by the amount of information that must be handled in order to create a structure–property relationship. The number of parameters required to describe the locations of N crystals in an aggregate with respect to a frame of reference is $3N$. An equiaxed grain in the form of a Kelvin tetrakaidecahedron will have fourteen faces, so that the number of bicrystal orientations that must be described per grain becomes $(1/2)\times 14\times 3N=21N$. Each of these interfaces will have two degrees of freedom so the parameters become $14\times 2\times 21N=588N$. A typical grain size is about $10\,\mu$m so a cubic centimetre of material will contain $N=10^{12}$ grains so that its full description requires about 10^{15} parameters! If the volume of each grain also needs to be specified than the problem become intractable.

There is no experimental technique available which can resolve all these parameters. Bulk measurements have for many decades been able to correlate both the texture and its intensity to a variety of properties. But in most cases these measurements neglect the location of crystals and also the interface planes; such neglect may not be important depending on the property being modelled. However, the EBSD technique offers more information in the sense that the microstructure can be viewed at the same time as the orientation of each crystal. Nevertheless, the observations of microstructure are on two-dimensional sections and hence do not give sufficient information about the orientations of interfaces. Serial sectioning methods help here but the amount of work involved to get meaningful statistics or accuracy in the context of engineering is impossibly large.

It is unlikely therefore, that engineering grain boundaries *per se*, as opposed to creating favourable textures, can be realised without (a) experimental methods to obtain large quantities of accurate information on the crystallographic indices of boundary planes and (b) methods for interpreting the resulting vast quantities of information. At this stage, it remains the case that most progress is made by manipulating orientations rather than boundaries. It is arguable whether, if it becomes possible to readily collect all the necessary information for grain 'boundary' engineering, we have the capability to exploit the quantities of data that emerge.[52)]

5. A Major Difficulty

Comparisons of calculated and measured textures as described above and in the published literature are misleading in the sense that 'intensities' are not calculated. It is only the positions of the poles which are calculated, assuming that each crystallographic variant contributes an exactly identical intensity to the overall texture. For example, an austenite grain containing two variants of martensite of equal size will display the same calculated texture as that in which one variant is a hundred times larger in volume than the other (**Fig. 7**).

To do a proper calculation requires not only the crystallography of each variant but also its volume, a problem which requires thermodynamic and kinetic theory to be incorporated into the texture calculation. In the case of displacive transformations, there has been one study of this problem,[27)] based on the assumption that it is the total free energy that a particular variant experiences which determines the extent of variant selection, although once the number of variants in any given austenite grain is established, they are all assumed to contribute equally.

The total free energy available for transformation is the sum of the chemical and mechanical components, the latter being zero in the absence of an applied stress during transformation[44,48)]:

$$\Delta G = \Delta G_{CHEM} + \Delta G_{MECH} \quad\text{.....................(7)}$$

where $\Delta G_{MECH} \equiv U$. It may be reasonable to assume that there is strong variant selection when the ratio of $\Delta G_{MECH}/\Delta G$ is large.[53)] This turns out to be the case as illustrated in **Fig. 8**. There is a strong, albeit empirical, linear correlation between the ratio $\Delta G_{MECH}/\Delta G$ and the number of most favoured variants allowed to form in each of the austenite grains.[27)] Although limited in its rigour, this is a useful observation in that it allows the extent of variant selection, and hence the transformation strains, to be calculated as a function of stress for any steel as long as the thermodynamic quantities can be estimated. This is an area where progress is needed from a fundamental point of view. When using this method, it is important to realise that the common assumption that $U=(1/2)\sigma_{ij}\varepsilon_{ij}$ is based on elasticity theory, and is therefore inappropriate when using Eq. (7).[55)] The strain due to transformation is plastic so the factor of 1/2 should not be there.

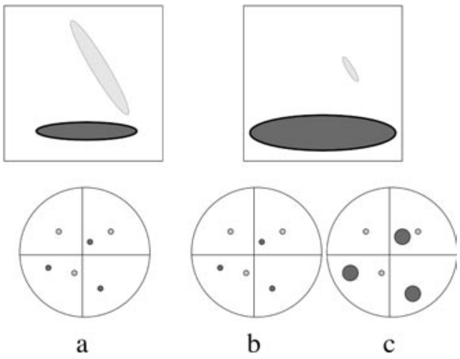

Fig. 7. Schematic illustration of the difficulty in calculating pole figures. (a) and (b) represent the pole figures calculated without taking account of the volume of the diffracting crystal, whereas (c) is meant to show intensity scaling with the fraction of the contributing crystals.

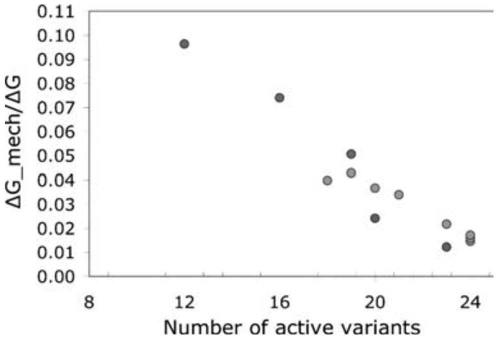

Fig. 8. $\Delta G_{MECH}/\Delta G$ *versus* the number of most favoured variants per grain (n), for a variety of steels.[27)] Data from.[27,47,54)]

6. Reconstructive Transformations: Lack of Theory

The crystallographic theory of martensite[29–31)] is probably the most complete formulation in the field of materials science, with its ability to describe every significant feature of a displacive transformation. The calculation of transformation texture therefore has a firm foundation in science. There is no equivalent model for reconstructive transformations, no established theory which allows the calculation of an orientation relationship, variant selection or transformation strains. The calculations generally begin by assuming an orientation relation but the product (α) is not confined to the grain in which it nucleates so a single ferrite grain can be in contact with many austenite crystals (Fig. 3).

Variant selection could be determined by any of the criteria listed below, all of which require much more information about the local environment than is currently available or possible to determine:

- When the α nucleates at a γ grain boundary, edge or corner, it may adopt a variant of the assumed orientation relationship which allows it to lattice match with the maximum number of austenite grains that it touches.
- The orientation of the austenite grain boundary plane with respect to the specific variant of the assumed orientation relationship may play a role in variant selection.
- External influence such as stress may be through its interaction with the isotropic volume change accompanying transformation (but is this more than a hydrostatic interaction?) or due to defects introduced by the stress. In the case of magnetic fields, particular variants may be favoured which have their magnetic domains better aligned to the field, as long as the transformation temperature is below the Curie point.
- It may be the case that nucleation occurs *via* the same atomic mechanism as displacive transformations, in which case the same theory might be used to establish orientation relationships. But this is not sufficient to determine the selection of variants since growth does not involve a shape deformation beyond the volume change, and the role of long-range diffusion has yet to be accounted for.

7. Summary

The most rigorous calculations of transformation texture are based on the crystallographic theory of martensite, which applies not only to martensite but also bainite and Widmanstätten ferrite. Here it is also possible to estimate variant selection and the resulting anisotropic transformation strains that develop on a macroscopic scale. It is emphasised, however, that although the methods allow the orientations to be predicted, they do not permit the volume fractions of particular variants to be estimated. The intensity of texture is not therefore predicted, only the locations of poles on a stereogram.

The situation regarding reconstructive transformations is much less developed and even the principles of variant selection are not yet established with confidence.

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