Comments on "The mechanisms of the fcc–bcc martensitic transformation revealed by pole figures"

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Abstract

It has been suggested in recent work that the observed spread in crystallographic orientations of martensite can be explained in terms of a new theory which attributes the effect to crystals which are at different stages in the evolution of martensite. We show here that this is mathematically incorrect and that the theory does not make predictions.

Key words: martensite, phenomenological theory, orientation relationships, electron back scatter diffraction, crystallography

In a recent paper [1] a theory is introduced for the martensite transformation. The work is inspired by the observation of spread in diffracted intensity within pole figures determined using electron back scatter diffraction (EBSD). The authors suggest that this spread is caused by "a trace of the transformation mechanism", resulting from the rotational parts of the transformation strain involved in a two-step $\gamma \rightarrow \varepsilon \rightarrow \alpha$ sequence, where the phases represent austenite, hexagonal close-packed martensite and body-centred cubic martensite. It is demonstrated in this letter that this theory is wrong, and that it does not explain the spread in diffracted intensity. Several incorrect statements made by the authors about the classical crystallographic theory of martensite [2–4] are also addressed.

The essential concept of the proposal can be explained without considering the two stages in the $\gamma \to \varepsilon \to \alpha$ reaction. The $\gamma \to \varepsilon$ transformation occurs by a shear **P** of magnitude $8^{-1/2}$ on the system $\{1\,1\,1\}_{\gamma} < 1\,1\,\overline{2} >_{\gamma}$. Note that **P** is strictly an invariant plane strain, i.e., there is also a dilatation normal to the $\{1\,1\,1\}_{\gamma}$ habit plane [5, 6]. **P** can be factorised into a pure deformation **Q**

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and a rigid body rotation \mathbf{R} [7]. For the $\gamma \to \varepsilon$ transformation, the principal deformations are less than, equal to and greater than 1, so that the operation of \mathbf{Q} leaves one line $(< 1\overline{10} >_{\gamma})$ undistorted and unrotated. The rigid body rotation \mathbf{R} occurs about this invariant axis, by a specific angle θ (10.03° dependent on lattice parameters [7]), which permits a second invariant line to be generated. These two invariant–lines result in an invariant plane, thus allowing the transformation to produce a coherent $\{111\}_{\gamma} | |(0001)_{\varepsilon}$ interface between the parent and product crystals.

Cayron et al. argue that the observed spread in orientations is partly explained by considering rotations about $\langle 1\overline{1}0 \rangle_{\gamma}$ with the rotation angle varying continuously between 0 and the 10.03° angle, the set of operations they label A^{α} . This is a crucial error because any rotation different from θ will not result in the coherent habit plane $\{111\}_{\gamma}$, nor in the correct shear deformation since $\mathbf{P} = \mathbf{RQ}$. It is wrong to consider the orientation relationship to be independent of the other crystallographic features of the transformation, i.e., the habit plane and shape deformation.

Note also that the theory [1] is not capable of making *predictions* of the observed pole figures since it contains only a qualitative proposal that the intermediate stages of transformation are locked into the microstructure.

A number of assertions are made about the classical crystallographic theory of martensite [2–4].

- It is argued that the Bain strain is associated with a large strain energy. What the authors fail to realise, in spite of statements made in the paper that the classical theory is phenomenological, is that the Bain strain is simply one component of the transformation strain. The total deformation is more complicated because it leads to a much lower strain energy. All of the components of the deformation occur at a moving interface. They do not occur in a sequence.
- The classical crystallographic theory predicts either twinning or slip as a lattice invariant deformation. It is claimed [1], that "slip steps nor twinning could be observed in many steels". We are not aware of any work where such features are not found when looked for with sufficient resolution.
- There is an extraordinary conclusion [1] that the shape shear implied by the classical theory has not been observed. There is a huge literature showing experimental measurements of the shape shear and its compatibility with the classical theory; for example, [8].

Some comments on pole figures. Diffraction from a perfect and large single crystal will occur under conditions which rather precisely satisfy the Bragg condition. This is not the case when the crystal is small or when it contains a significant density of defects which disrupt the long-range periodicity of the atomic arrangement. The fine martensite which occurs in low-alloy steels, such as the one considered in [1], contains excess dislocations leading to a spread in diffracted intensity. Furthermore, the contribution to the spread from different crystals of 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. As a consequence, the measured distribution of intensity on a pole figure will not be sharp and indeed, it is usual to express such diffuse scattering using intensity contours. Superimposed on the strain and size broadening will be the effect of experimental error in the EBSD detection system. In the case of the plots reported in [1] there will be an additional and unspecified error in reconstructing the austenite orientation from that of martensite. Although the authors have not indicated the composition and heat-treatment of the "9Cr" steel studied, such an alloy is usually severely tempered [9] after martensitic transformation which means that there will be orientation changes due to recovery and the motion of boundaries. The same applies to the meteorite studies [10] which are referred to in [1], where the cooling rates from the transformation temperature are incredibly slow.

In summary, the concept described by Cayron et al. does not seem to be correct from a crystallographic point of view, and it is incapable of making predictions about the observed pole figures.

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