Crystallographic Texture and Intervening Transformations

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Abstract: We examine here the case that in deformed austenitic stainless steels, the transformation texture should be calculated in two–stages [1]. The first involves the transformation of austenite into ϵ–martensite, which then changes into body–centred cubic martensite. The procedure requires two fitting parameters, connected with the extent of variant selection. Our analysis shows that it may not be necessary to follow this procedure, with the texture adequately calculated by considering direct transformation into body–centred cubic martensite. Some comments are also made about the calculation of the interaction energy between the applied stress and martensite.

Keywords: Transformation texture, martensite, stainless steel, stress–affected transformation

In a recent study the crystallographic texture of an austenitic stainless steel which transformed into body–centred cubic martensite (α') during deformation, was calculated in two stages [1]. The austenite was considered first to transform into the hexagonal close–packed ϵ-martensite which then evolved into α' martensite. Other work has suggested that the $\gamma \rightarrow \alpha'$ transformation occurs in two stages [2, 3].

A different approach was also used to calculate the interaction energy between the applied stress and the transformation strain [1], based on elasticity theory rather than the plastic work model of Patel and Cohen [4].

The purpose of the present work was to see whether it is in fact necessary to account for ϵ-martensite when estimating the transformation texture due to α'. There may not be an *a priori* reason to suppose that anything but the total deformation due to $\gamma \rightarrow \alpha'$ can influence the ultimate selection of α' variants.

Transformation texture arises because not all possible crystallographic variants grow when the austenite is subjected to external stress. The interaction between the stress and the shape deformation of the martensite is represented mathematically by calculating an interaction energy. A second aim therefore was to assess the energy criteria used in variant selection during stress–induced martensitic transformation.

Consistent with the approach used in [1], we assume that the transformation can be described as being 'stress–assisted' rather than 'strain–induced'. This assumption relies on the observation that the texture for the small tensile strain (10%) involved [1], the texture can in practice be calculated assuming that variant selection depends only on the interaction of stress with the shape deformation of the martensite [5]. It should also be noted that much larger plastic deformations are needed before effects such as mechanical stabilisation of martensite become prominent in type of steel considered here [6, 7].

The shape deformation due to martensitic transformation is an invariant–plane strain on a plane with a unit normal $(\mathbf{p}; \gamma^*) = (\mathrm{p}_1\ \mathrm{p}_2\ \mathrm{p}_3)$, a displacement in the unit direction $[\gamma; \mathbf{d}] = [\mathrm{d}_1\ \mathrm{d}_2\ \mathrm{d}_3]$ of magnitude m. The terms γ and γ^* define the real and reciprocal bases of the austenite and bold symbols refer to vectors; p_i and d_i are components of $\mathbf{p}$ and $\mathbf{d}$ respectively. The notation used here is due to Bowles and MacKenzie [8]. The deformation can be represented by a matrix $\mathbf{P}$ in the austenite basis as follows [9–11]:

$$(\gamma\ \mathrm{P}\ \gamma) = \begin{pmatrix} 1 + m\mathrm{d}_1\mathrm{p}_1 & m\mathrm{d}_1\mathrm{p}_2 & m\mathrm{d}_1\mathrm{p}_3 \\ m\mathrm{d}_2\mathrm{p}_1 & 1 + m\mathrm{d}_2\mathrm{p}_2 & m\mathrm{d}_2\mathrm{p}_3 \\ m\mathrm{d}_3\mathrm{p}_1 & m\mathrm{d}_3\mathrm{p}_2 & 1 + m\mathrm{d}_3\mathrm{p}_3 \end{pmatrix} \tag{1}$$

Since $\mathbf{P}$ is a *plastic* deformation which does not in steels relax on the removal of stress, the interaction energy in the Patel and Cohen method [4] is simply the $(\sigma_N \times \delta) + (\tau \times s)$, where σ_N is the normal stress on the invariant–plane, δ is the dilatational strain along $\mathbf{p}$, τ is the shear stress on the invariant–plane in the direction $\mathbf{e}$, Fig. 1, and s is the shear strain along the unit vector $\mathbf{e}$.
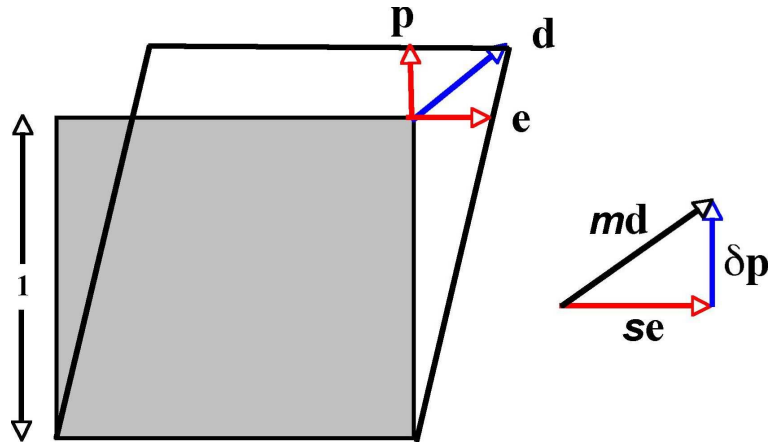

Fig. 1. Shape deformation associated with the martensite transformation. Austenite is shaded grey.

For a given system of stresses expressed as a stress tensor, one would have to resolve the

traction $\boldsymbol{\sigma_t}$ on the invariant–plane into the normal and shear stresses as follows:

$$\boldsymbol{\sigma_t} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \tag{2}$$

The normal stress on the invariant–plane is then given by $\sigma_N = \boldsymbol{\sigma_t} . \mathbf{p}$. The shear stress on the invariant–plane in the direction $\mathbf{e}$ is $\tau = (\boldsymbol{\sigma_t} - \boldsymbol{\sigma_N}) . \mathbf{e}$. For a stress tensor in the basis γ, representing a uniaxial stress ($\sigma_{11} = \sigma$ and all other components zero), it follows that the interaction energy is

$$U = md_1 p_1 \sigma \tag{3}$$

The alternative method of calculating the interaction energy relies on elasticity theory [1, 12]:

$$\begin{aligned} U &= \frac{1}{2}\sigma_{ij}\epsilon_{ij} \\ &\equiv \frac{1}{2}[\sigma_{11}\epsilon_{11} + \sigma_{22}\epsilon_{22} + \sigma_{33}\epsilon_{33} + \sigma_{12}\gamma_{12} + \sigma_{13}\gamma_{13} + \sigma_{23}\gamma_{23}] \\ \text{with} \quad \epsilon_{ij} &= \frac{(\gamma \ P \ \gamma) + (\gamma \ P' \ \gamma)}{2} - I \end{aligned} \tag{4}$$

and for the case of uniaxial tension discussed earlier, gives an interaction energy

$$U' = \frac{1}{2}md_1 p_1 \sigma \tag{5}$$

This differs by a factor of 2 from equation 3, because the latter incorrectly assumes that the stress-strain relationship is elastic whereas in fact the transformation strain is plastic. That this conclusion is generic can be seen as follows, for a general stress tensor (summation convention applies):

$$\begin{aligned} \boldsymbol{\sigma_N} &= (\sigma_{ij}p_i p_j)\mathbf{p} \\ \tau &= (\boldsymbol{\sigma_t} - \boldsymbol{\sigma_N}) . \mathbf{e} = \sigma_{ij}p_j e_i \\ U &= [\delta\sigma_{ij}p_i p_j + s\sigma_{ij}e_i p_j] = \sigma_{ij}p_j[\delta p_i + s e_i] \\ &= \sigma_{ij}p_j m d_i \\ &\equiv \sigma_{ij}\epsilon_{ij} \end{aligned} \tag{6}$$

Both methods will give exactly the same ranking of interaction energy when different crystallographic variants are considered. However, the absolute value of U is important because it has to be compared against the chemical driving force $\Delta G = G_\gamma - G_{\alpha'}$ for transformation [13]. Variant selection is unlikely when $U \ll \Delta G$. In these circumstances, the model of Patel and Cohen [4] is strictly the correct procedure to use since the transformation strain is plastic.

We now examine experimental data [1] on texture evolution in austenitic stainless steel.

The general criterion that the most favoured crystallographic variant is associated with the highest interaction energy is a reasonable starting point for any texture calculation. One possibility is to assume that all variants with a favourable U are allowed in the calculation. Another procedure introduces an arbitrary cut–off in a manner consistent with observations. In a two–stage $\gamma \to \epsilon \to \alpha'$ reaction it would be necessary to make two such arbitrary cut–offs, one each for the ϵ and α'.

For the $\gamma \to \epsilon$ transformation Humbert *et al.* assumed "strong" variant selection, *i.e.,* all variants with an interaction energy less that 90% of the maximum value were not allowed to form. For the $\epsilon \to \alpha'$ transformation the threshold for rejecting variants was 20% of the maximum value in order to obtain a match with experimental data. Given these fitting parameters, the closure between experiments and calculations is illustrated in Fig. 2. Some of the data (marked black) are not reproduced by the calculations.
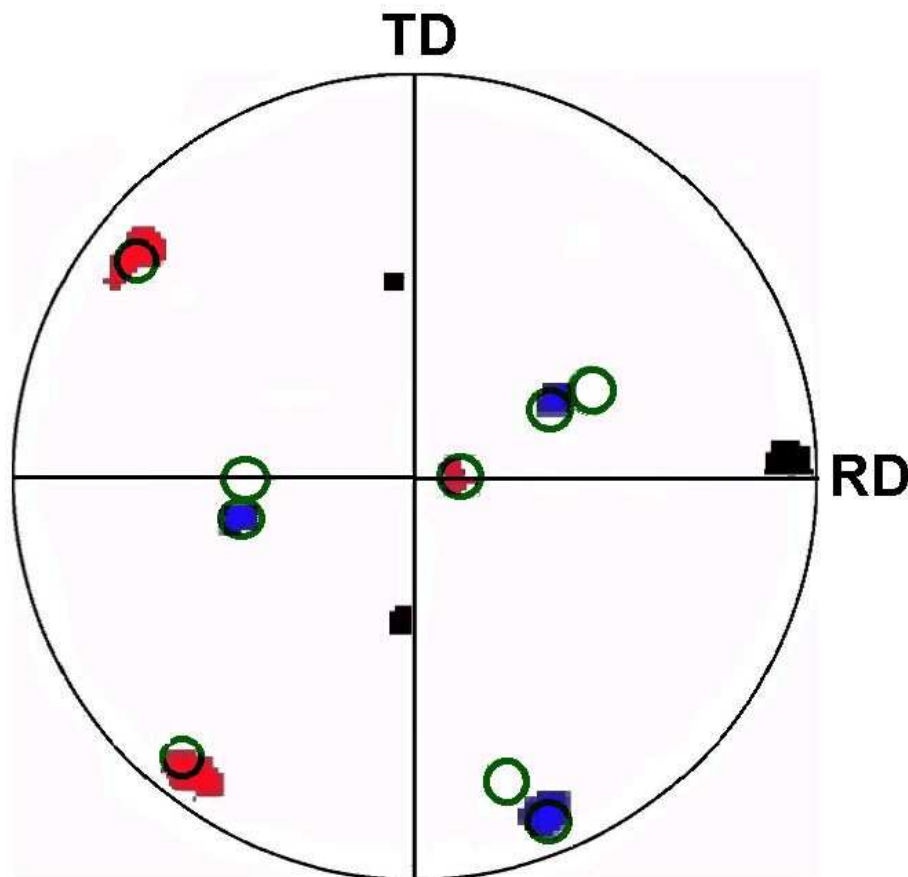

Fig. 2. 1 0 0 pole figure of α' martensite for an austenite grain in an orientation defined by the Euler angles $[128.99°, 48.27°, 24.27°]$. All data from Humbert *et al.* [1]. The measured data are in three orientation groups identified by their different colours, whereas the calculated data are represented by circles.

Suppose it is assumed now that the α' transformation texture can be calculated without accounting for the ϵ. The resulting interaction energies, for the same austenite grain orientation as in [1], for the 24 possible variants of martensite are listed in Table 1. The crystallographic data used to define the α' are shown in Table 2, obtained following the procedure described

Table 1
Calculation of interaction energy associated with $\gamma \to \alpha'$ transformation following Patel-Cohen [4].

Ranking	Variant No.	Interaction energy / J mol^{-1}	Ranking	Variant No.	Interaction energy / J mol^{-1}
1	2	110.64	13	11	5.70
2	10	108.68	14	4	-4.72
3	21	100.36	15	13	-9.68
4	20	88.80	16	5	-18.51
5	3	79.43	17	16	-22.90
6	8	72.52	18	14	-36.34
7	23	61.11	19	7	-45.22
8	18	60.21	20	6	-52.25
9	19	59.17	21	9	-74.18
10	24	41.87	22	12	-86.10
11	17	37.87	23	15	-106.72
12	22	23.94	24	1	-120.73

Table 2
Crystallographic data set for α' martensite in 304 stainless steel.

Habit plane	$(-0.183989\ 0.596344\ -0.781359)_\gamma$
Shape deformation matrix $(\gamma\ P\ \gamma)$	$\begin{pmatrix} 0.991342 & 0.028064 & -0.036770 \\ 0.028064 & 0.909040 & 0.119180 \\ 0.029429 & -0.095386 & 1.124979 \end{pmatrix}$
Coordinate transformation matrix $(\gamma\ J\ \alpha)$	$\begin{pmatrix} 0.579356 & 0.542586 & 0.102537 \\ 0.014470 & 0.133650 & -0.788984 \\ -0.552000 & 0.572979 & 0.086936 \end{pmatrix}$

in [11].

The first 13 variants listed in Table 1 all have a positive interaction energy and hence are favoured by the applied stress. Fig. 3 shows the comparison between experimental and model predicted $1\ 0\ 0_{\alpha'}$ pole figure, assuming that all variants for which $U > 0$ can grow. The locations of all the observed intensities are explained approximately using this procedure. Note that both the theoretical analysis [1] and the present work is not able to predict intensities, but rather the locations where intensity is expected. And when presenting experimental data, the appearance of the pole figure depends on thresholds set to reject noise from signal. On this basis, the agreement between the expected and actual positions illustrated in Fig. 3 is

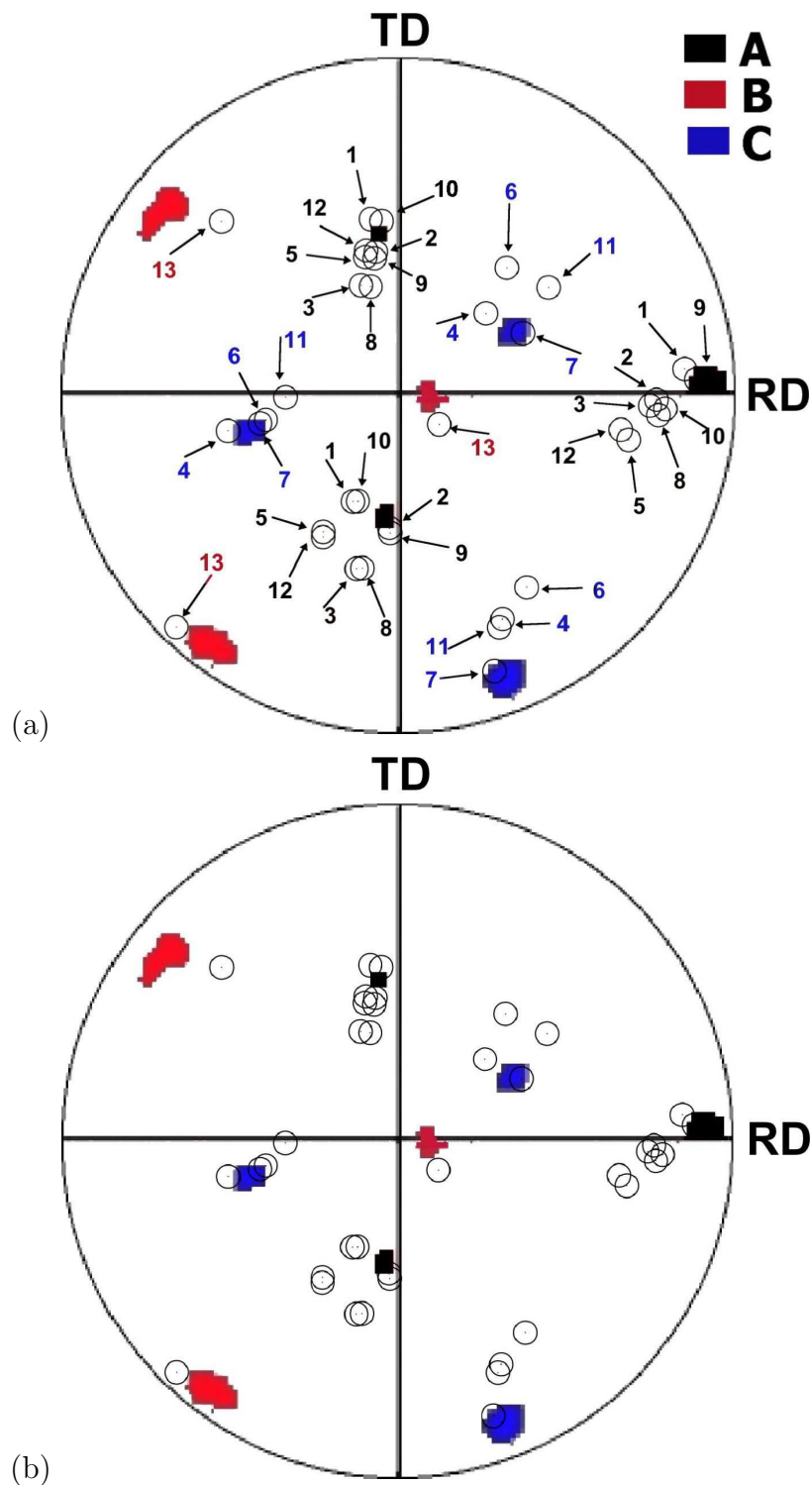not unreasonable, especially since no attempt has been made to fit the data.

Fig. 3. Model predicted 1 0 0$_{\alpha'}$ pole figure for α' martensite. Coloured areas corresponds to experimental observation of Humbert *et al.*. Open circles represent model predictions. (a) Shows the details of predicted variants, (b) without detail.

It has already been demonstrated that the polycrystalline–austenite texture data in [1] are

well–predicted using the simple $\gamma \rightarrow \alpha'$ path [5].

To summarise, it does not appear necessary to consider a two–stage transformation of austenite, first into ϵ-martensite which then changes to α'-martensite, in order to estimate the transformation texture in austenitic stainless steel. Indeed, the stepwise calculation introduces additional fitting parameters without which the texture cannot be predicted. Reasonable agreement between calculations and measurements is obtained by directly calculating the transformation texture for the $\gamma \rightarrow \epsilon$ reaction, although it has to be emphasised at the same time that better experiments are needed in two respects. First, the quantitative measurement of fractions of different variants within given austenite orientations, and secondly the crystallographic set describing martensitic transformation needs verification for the system of interest.

The ranking of interaction energies in the single step analysis proposed here should be equivalent to the final ranking obtained in the two–step process, as long as the selection are made without bias. This latter point cannot be guaranteed in [1] since there are arbitrary thresholds set for rejecting variants at each of the two stages, whereas we simply select all variants with positive interaction energies.

It is important to note that the methods for texture calculation described here and elsewhere deal primarily with the location of crystallographic poles in a polycrystalline sample, rather than the number density of those poles in crystallographic space. To define the latter requires a criterion which includes both the mechanical and chemical free energy components defining martensitic transformations, the former being the interaction energy between the shape deformation and applied system of stresses. In this case, the correct magnitude of the interaction energy should be calculated according to Patel and Cohen [4] since the shape deformation is a plastic strain. An elasticity approach will make this value incorrect by a factor of two.

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