Symmetry breakdown related fracture in steel

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Abstract

Crystallographic orientation symmetry in 42CrMo4 steel austempered below martensite start temperature was investigated with the help of the ODF analysis based on FEG-SEM/EBSD technique. The results, verified by simple modeling, show straightforward that under plane-strain conditions cracks prefer to propagate through areas where the crystallographic orientation symmetry was broken.

Keywords: Modeling; Texture; EBSD; Austempering; Bainite; Fracture

Graphic abstract

SYMMETRY BREAKDOWN

IDEAL SYMMETRY

FRACUTRED
As described by Biezeno and Grammel in 1953 [1], if the crack is free to propagate along a certain path, it must choose that path which minimizes the Lagrangian function, the stable solutions of which exhibit less symmetry than the equation itself, hence releases the maximum energy from the system. This is true for dynamic as well as quasi-static crack propagation [2]. In this sense, fracture could be either a consequence or an origin of spontaneous symmetry breaking, a very common occurrence in physics. In the present consideration, the resistance to crack propagation is vital for industrial applications of ultrahigh-strength low-alloy (USLA) steel such as 42CrMo4 (AISI 4140, DIN/EN 1.7225) heat treated to have a yield strength over 200 ksi (1379 MPa) [3]. After spontaneous phase transformation, high crystallographic symmetry especially sixfold orientation symmetry could as a matter of fact always be present in these steel [4]. However, the effect of crystallographic orientation symmetry and/or symmetry breakdown on the overall properties of steel in particular fracture, which could be significant, is still unknown. In order to figure out this problem, both experimental and theoretical investigations are performed.

The chemical composition and metallurgical features of the versatile 42CrMo4 steel are represented in Table 1. The cycles of heat treatment, the preparation of circumferentially notched round bars and the performance of the notched tensile testing have been described elsewhere [5]. Cracks were introduced by the notched tensile testing interrupted right before the load reached the average notched fracture load. Crystallographic orientations of the microstructure of various specimens were measured at room temperature by FEG-EBSD technique and analyzed by MatLab-MTEX toolbox. The accelerating voltage for EBSD measurements was 20 kV, the step size was 100 nm, and the tolerance range of the Euler-angle measurements is $0.5 \sim 1^\circ$ in these observations. The overall hit rate was $> 80\%$, which is approx. 10% lower than the measurements on specimens uncracked.
Table 1. Chemical composition (in wt.%) of 42CrMo4 steel investigated; volume fraction of retained austenite \( (f_{RA}, \text{in } \%) \), effective grain size \( (d_{eff}, \text{in } \mu \text{m}) \) and aspect ratio \( (\kappa', \text{in } -) \) of lath-shaped blocks in 42CrMo4 steel austempered below \( M_S \). w.a. refers to weighed by area and w.l. weighed by length, respectively.

| C  | Si | Mn | S  | P  | Cr | Mo | Fe | \( f_{RA} \) | \( d_{eff} \) \(^a\) | \( \kappa' \) \(^b\) |
|----|----|----|----|----|----|----|----|------------|-------------|----------|
| 0.40 | 0.35 | 0.82 | 0.018 | 0.007 | 0.90 | 0.11 | Bal. | 0 | 2.5 | 0.9 | 0.4 | 0.4 |

\(^a\) Estimated with the maximal misorientation angle of 15°.

\(^b\) Peak position, fitted by the Pseudo-Voigt function.

Fig. 1 shows the inverse pole figure (IPF) map of the representative quasi-homogeneous microstructure on the plane-strain crack path. The lath-morphology of the microstructure retains in the IPF maps, even after the recalculation of EBSD maps with the maximal misorientation angle of 15°. Experimental ODF was rotated to show the symmetry about the \((111)\). Area I displays a sixfold symmetry, as shown in Fig. 2b, which compares to the ideal sixfold symmetry as represented in Fig. 2a. Area II displays a strongly deformed sixfold symmetry (Fig. 2c). Strong \((110)\) orientations appear on the great circle of ODF in the plane-strain cracked Area III, leading to a strong offset of the sixfold symmetry (Fig. 2d).

Fig. 3 represents the ODF sections for Area I, II and III in Fig. 1, calculated on the basis of a cubic crystal and monoclinic sample symmetry from the \{111\} complete pole figures. The monoclinic symmetry delivers here the most stable and distinguishable texture components. As crystallographically components \((E1\) and \(E2\)) and \((J1\) and \(J2\)) cannot appear independently for monoclinic symmetry, in the analyses and discussion that follow distinctions will not be made between them. The observed b.c.c. texture components are listed in Table 2. In Fig. 3a, the only major orientation evident is \(J\). The remaining major orientations \(D1, D2,\) and \(F\) are practically absent. The intensity of \(E\) is approximately half that of \(J\). In Area II visible are the major orientations \(D1, E, F, J,\) and the transformation texture \((110)[1-10]\). In particular, the intensity of \((110)[1-10]\) compares to that of \(J\), while the intensity of \(D1\) is approximately half that of \(D2\) (Fig. 3b). In plane-strain cracked Area III, the intensity of \((110)[1-10]\) is approximately
twice that of D2, E, F, and J. The \{110\}b fiber extends from F through J to E along the \(\varphi_2\) direction (Fig. 3c).

Fig. 1. Inverse pole figure (IPF) coloring of fractured microstructure with lath-shaped blocks in 42CrMo4 steel austempered below \(M_S\). Colors of crystals agree with the orientations perpendicular to the observed plane, which is indicated in the stereographic triangle.
(a) Ideal sixfold symmetry, (b) well evident sixfold symmetry in Area I, (c) strongly deformed sixfold symmetry in Area II, and (d) sixfold symmetry is undetectable in cracked Area III.

Table 2. Description of observed b.c.c. texture components developed either directly by shear (S) or by the transformation of sheared austenite (T).

| Symbol | Component | Type | Shear   |
|--------|-----------|------|---------|
| J1     | (0-11)[-211] | S / T | 0.11 – 0.58 |
| J2     | (1-10)[-1-12] | S / T | 0.11 – 0.58 |
| D1     | (11-2)[111] | S / T | 0.07 – 0.29 |
| D2     | [-1-12][111] | S / T | 0.94 |
| E1     | (01-1)[111] | S / T | 0.09 – 0.81 |
| E2     | (0-11)[111] | S / T | 0.09 – 0.81 |
| F      | (110)[001] | S / T | 0.05 – 0.09 |
| Cα     | (110)[1-10] | T     | 0.58 |

*Dependent on the parent components of the γ-α transformation.

Fig. 3 indicates areas with the broken symmetry may crack first, whereas areas with near ideal symmetry can hold in the plane-strain state. Only if, the observed break of the symmetry should not be developed by shear of the b.c.c mixed microstructure, but rather directly by the spontaneous phase transformation of sheared f.c.c austenite. In the other words, the following statement must be proven: it is the broken symmetry that weakens the materials and it is not the plastic deformation or even failure of the material that breaks the symmetry. The observed development of the texture as shown in Fig. 3 implies that this statement is indeed legal. A switch of the dominant texture components from J to (110)[1-10] has been observed in Area I to III. The (110)[1-10] components have been emphasized in Area II and dominate in Area III, changing the symmetry of these areas significantly. As demonstrated in Table 2, the (110)[1-10]
components are developed directly by the spontaneous transformation of sheared f.c.c austenite, which has been preliminarily analyzed by Wittridge and Jonas [6]. As a result, it can be concluded that the spontaneous transformation components break the symmetry and the plane-strain fracture toughness of the material deteriorates.

Fig. 3. Measured deformation and transformation textures of (a) Area I, (b) Area II, and (c) Area III with monoclinic symmetry.
In the theoretical modeling following assumptions are made:

A. The crack through the fractured subunits obeys elastic-plastic fracture mechanics (EPFM) and has a plastic zone upon the plane-strain condition.

B. The inter-subunit fracture is insignificant after austempering below martensite start temperature (ABMS).

C. The radius of the selected integration contour for the path-dependent $J$-integral is quantized by the average effective path of the crack propagating through individual subunits.

D. A uniform distribution of the crystallographic symmetry of grains is assumed.

The boundary of the plastic zone is a function of $\theta$, i.e. the angle between the radius of the plastic zone and the propagating direction of the crack tip. For a plane-strain case, it is well known

$$ r(\theta) = \frac{1}{4\pi} \left( \frac{K_I}{\sigma_y} \right)^2 [ (1 - 2\nu)^2 (1 + \cos \theta) + \frac{3}{2} \sin^2 \theta ] $$

where $\sigma_y$ is the yield strength, $K_I$ the stress intensity factor, and $\nu$ the Poisson's ratio. Obviously,

$$ r(\theta) \leq \frac{\eta}{4\pi} \left( \frac{K_I}{\sigma_y} \right)^2 $$

i.e.

$$ r_y = \frac{\eta}{4\pi} \left( \frac{K_{IC}}{\sigma_y} \right)^2 $$

with

$$ \eta = \frac{3}{2} (1 - 2\nu)^2 + \frac{1}{6} (1 - 2\nu)^4 $$

Beyond the maximal radius of the plastic zone $r_y$, the selected integration contour for $J$-integral is greater than the plastic zone size and $J$-integral becomes path-independent.

After assumption C, it yields

$$ r_y = fL $$
where $f$ is the frequency of crack propagation, say, $f = \phi/c$ for qualitative discussions. Here $\phi$ is an experimentally accessible and material-dependent length parameter. Upon assumption D, it is then possible to calculate the average crack propagation length $\bar{L}$ on an 2D-intersection of a 3D-martensitic/bainitic ellipsoid in the form of an ellipse of major-axis $a$ and minor-axis $c$, with $a \gg c$ and $\kappa = c/a$. $\bar{L}$ can be simultaneously treated as the quantized energy needed to cut through ellipsoids and calculated from $(N-1)$th root of the $(N-1)$th products of chord lengths of an ellipse

$$
\bar{L}^{N-1} = \frac{N}{c} \left[ \left( \frac{a + c}{2} \right)^N - \left( \frac{a - c}{2} \right)^N \right] = \frac{N}{2^N c} [(a + c)^N - (a - c)^N].
$$

Here $\bar{L}^{N-1}$ is $N/c$ times the $N$th Fibonacci number and $N$ is called the geometric number controlled by the transformation symmetry of substructure with $N \in \mathbb{N}$ and $N \gg 2$.

By combining Eq. (3) to (6), it yields

$$
K_{IC} = \sigma_y \omega \sqrt{\frac{2 \pi \phi}{\eta}}
$$

with

$$
\omega = \left\{ \frac{N}{2} \left[ \left( \frac{1}{\kappa + 1} \right)^N - \left( \frac{1}{\kappa - 1} \right)^N \right] \right\}^{1/[2(N-1)]}.
$$

After the binomial expansion, Eq. (7) turns to

$$
K_{IC} = \sigma_y \sqrt{\frac{2 \pi \phi}{\eta}} \left[ \sum_{k=1}^{m} \frac{N}{2k - 1} \frac{1}{\kappa^{N-(2k-1)}} \right]^{1/[2(N-1)]}
$$

with $\exists m \in \mathbb{N}:(N+1)/2=m$.

By evaluating the limit of Eq. (9), it yields

$$
\lim_{N \to 2} K_{IC} \geq 2 \cdot \lim_{N \to \infty} K_{IC}
$$

with $\sigma_y^{N \to 2} \geq \sigma_y^{N \to \infty}$ owing to the strengthening effect of the high symmetry.
Obviously, upon constant $\kappa$, $\omega$ increases monotonically with decreasing $N$. If $N$ is small (but still $\gg 2$), only certain energetic pathways of the crack, which are constrained/controlled by the symmetric equivalent orientations, can be selected. On the contrary, as $N$ approaches infinity, the propagation of the crack turns unconstrained and the pathways of the crack across the subunits become random. The simple modelling shows that constraints induced by geometric symmetry can enhance the fracture toughness, whereas symmetry breakdown deteriorates $K_{IC}$. The experimental $K_{IC}$ values reported in the previous work [5] lie exactly between the threshold values predicted by Eq. (9) with the packet size as the selected value of $\phi$.

In summary, statistic ODF analysis with inverse pole figure maps was used to account for the crystallographic symmetry breakdown in 42CrMo4 steel austempered below $M_s$. Fracture toughness and crystallographic orientation symmetry were connected together by EPFM. The results of experimental studies, explained by the modeling, show that symmetry breakdown deteriorates $K_{IC}$ and/or facilitates fracture. The present work shows a remnant of a deep symmetry of the materials laws that are hidden from sight and could be of universal significance for understanding the fracture behavior of steel transformed at low temperatures.

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