Quantitative prediction of transformation texture in steel by Double Kurdjumov-Sachs relation

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Abstract. The transformation texture prediction by so-called double K-S relation is described. Various types of transformation textures such as the one in hot-rolled steel sheets and those of texture memory in hot-rolled steel and cold-rolled pure iron have been reported to be able to be quantitatively predicted by this variant selection rule. Recently such an experimental investigation has been extended to the texture memory in ECAP-processed pure iron. Although the type of texture as well as the symmetry of samples in ECAP iron is very different from the previous materials, the investigation has clearly indicated that the double K-S relation should indeed be the mechanism governing variant selection on the phase transformation in iron and steel.

1. Introduction

To develop new products in steel industry, it is desired to develop through-process texture simulation methods, since crystallographic texture largely influences the formability as well as elastic and magnetic properties of steels. However, the development of such a prediction method has been hampered by insufficient understanding of the mechanisms that govern the texture change during the manufacturing processes.

One of the phenomena on texture prediction that have long been investigated but not sufficiently understood is the transformation texture. During the phase transformation, the texture of parent phase is inherited to the texture of product phase due to the orientation relationship such as Kurdjumov-Sachs (K-S) relation [1] for the austenite (γ) to ferrite (α) transformation, $\{111\}_\gamma//\{011\}_\alpha$ and $<110>_\gamma//<111>_\alpha$. Then according to the orientation relation, the orientations in the parent crystals are rotated to develop the texture in product crystals. Therefore the prediction of transformation texture is seemingly rather straight forward. However, the prediction has been still only qualitative, since it is still unclear which of the variants in the orientation relation (24 for K-S relation) are preferentially selected. Understanding of such a variant selection is certainly indispensable to construct the models for through-process texture prediction. In this respect, we have proposed a variant selection rule that we call the “double K-S relation” [2, 3]. This mechanism relies on the nucleation of the product phase that preferentially occurs on grain boundaries of the parent phase, holding K-S relation or the one near it with adjoining two parent grains at the same time. In other words, the nucleation needs two parent grains having the K-S or near K-S relation. With this variant selection mechanism, the ferrite textures of hot-rolled steel [2] and the texture memory in the hot-rolled steel and cold-rolled pure iron [3] have been quantitatively predicted so far. In this article, the most recent experimental verification of the double K-S relation by observing in-situ the texture memory in the ECAP (equal channel angular pressing) -processed pure iron by pulsed neutron diffractometer HIPPO in Los Alamos Neutron Science Center [4] is described.

2. Texture prediction method and variant selection model

Although the calculation of change in texture during transformation becomes rather complicated if many variants operate at different probabilities, it can be calculated by the equations based on the spherical harmonic expansion of ODF (orientation distribution function) as shown below [5],

$$ {}^{P}C_{\lambda}^{\mu\nu} = \sum_{\lambda_1=0}^{\infty} \sum_{\mu=1}^{M(\lambda_1)} \sum_{\nu 1=1}^{N(\lambda_1)} {}^{M}C_{\lambda_1}{}^{\mu\nu_1} \left[\sum_{\lambda_2=0}^{\infty} \sum_{\nu_2=1}^{N(\lambda_2)} \sum_{m=-\lambda}^{\lambda} \sum_{s=-\lambda}^{\lambda} \rho_{\lambda_2}^{r\nu_2} \dot{A}_{\lambda_1}^{m_1\mu}(\lambda_1\lambda_2 mr \mid \lambda s)\{\lambda_1\lambda_2\nu_1\nu_2 \mid \lambda\nu\} \dot{T}_{\lambda}{}^{\mu s} * (\Delta g) \right] \quad (1) $$

$$ s = m + r, \qquad \left|\lambda_2 - \lambda_1\right| \le \lambda \le \left|\lambda_2 - \lambda_1\right|, \qquad s \le \lambda, \quad (2) $$

where ${}^{P}C_{\lambda}{}^{\mu\nu}$ and ${}^{M}C_{\lambda}{}^{\mu\nu}$ are the series expansion coefficients of the ODF's of product and parent phases respectively. The Δg represents the crystal rotation due to the K-S relation, and $\rho_{\lambda 2}{}^{\mu,\nu 2}$'s are the expansion coefficients of the variant selection function $\rho(g)$.
In this study, $\rho(g)$ is derived from the double K-S relation [2, 3]. To satisfy the double K-S relation, an α particle, which nucleates on the grain boundary having the i-th K-S relation to γ_1 (with orientation g) as shown in Fig.1, has to hold the K-S relation to γ_2 on the opposite side as well. Therefore if such K-S related γ_2 abundantly exists in the parent phase, the possibility for the i-th K-S variant to operate would become large. Hence such probability should be in proportion to the probability to find such K-S related γ_2 in the parent texture. Then, as described elsewhere [3], $\rho(g)$ is derived as follows,

$$ \rho(g) = \frac{\omega}{N} \sum_{k} f(\Delta g^{-1} \cdot g_k^c \cdot \Delta g \cdot g) + \rho_C(g), \quad (3) $$

where f(g) is the ODF of the parent phase, and $g_k{}^c$'s are the 24 rotational operators for the cubic symmetry group. Note that the variant selection is entirely determined by the texture of parent phase.

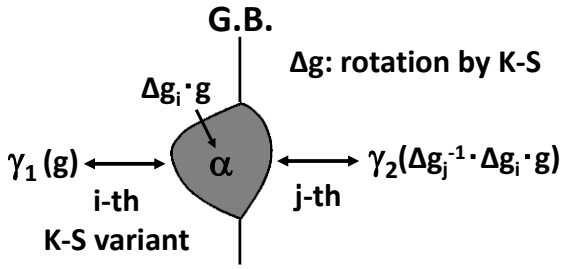

Fig.1 Schematic representation of double K-S relation

It should be also emphasized that we assume at least one of the K-S relations with the two neighboring parent grains to be allowed to deviate up to about 10° from the exact K-S relation. With this deviation allowed, the double K-S relation can occur on ordinary grain boundaries in ordinary parent structures. The proper value of the only parameter ω in Eq. (3) is known to be from 0.6 to unity for the transformation during hot-rolling processes in steel [2,3].

3. Verification using the texture memory in ECAP-processed pure iron

The texture memory effects, in which an initial texture is well retained after two transformations on heating and cooling ($\alpha \rightarrow \gamma \rightarrow \alpha$ in iron and steel), are thought to be ascribed to variant selection. However the selection mechanism has not been clarified thoroughly. If the double K-S relation is a universal property for the phase transformation between α and γ, such a memory effect should be explained thereby. Therefore the texture memory effects in different types of material have been observed by pulsed neutron diffraction and examined based on the double K-S relation. Here, such investigation using ECAP-processed pure iron is described. A rather different texture as well as symmetry of samples in the ECAP iron than before [2,3] particularly makes this investigation significant. The experimental results on this ECAP-processed iron have been published elsewhere [6].

3.1 Experimental

A 99.98% pure iron ingot was hot-forged and machined into a 25 x 25 x 170 mm^3 square bar and processed by ECAP at room temperature using the route B_c. The ECAP die had an internal angle (Φ) of 90°. The pressing speed was 2.5 $mm \cdot s^{-1}$. The von Mises equivalent strain

per pass is 1.15, corresponding to a total strain of 9.2 after 8 passes. Then in-situ pulsed neutron diffraction texture measurements were performed on HIPPO at LANSCE using a 8 mm-edge cube cut out from the central part of the ECAP-processed bar. Measurements were performed in vacuum at 50 and 800 ˚C on heating, at 950 ˚C after completion of $\alpha \rightarrow \gamma$ transformation and at 800 ˚C on cooling to measure the entire cycle of texture change during the $\alpha \rightarrow \gamma \rightarrow \alpha$ transformation. Heating and cooling rates were about 10 ˚C·min^{-1}. The dwell time at each temperature to acquire the data for texture analysis was about 5 min. The neutron diffraction data at each temperature were analyzed by simultaneous Rietveld analysis and a harmonics expansion method to reconstruct pole figures and ODF. Note that ODF's were calculated using different coordinates than those in ref. 6.

3.2 Experimental results and comparison with prediction based on the double K-S relation
The observed (111) pole figures of the ECAP-processed iron are shown in Fig. 2. Since the deformed structure by ECAP recrystallizes on heating, a large change is seen between the pole figures at 50 and 800 ˚C (Figs. 2(a) and (b)). Then it changes again by phase transformations from α to γ and from γ to α as shown in Figs. 2 (b) to (d). Although somewhat weakened, texture memory is apparent in those pole figures with the almost identical peak positions seen in Figs. 2 (b) and (d).

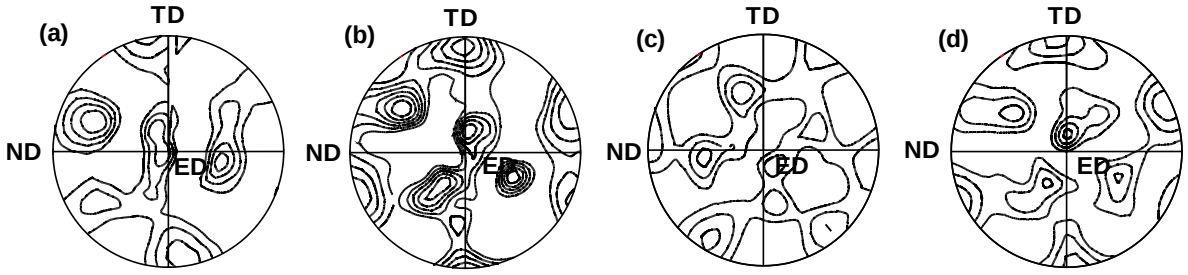

Fig. 2 Experimental (111) pole figures of ECAP-processed pure iron (a) at 50 ˚C (as deformed), after heating to (b) 800 ˚C and (c) 950 ˚C, and (d) after cooling to 800 ˚C; (a), (b) and (d) are for α, while (c) is for γ. Levels are 1.0, 1.2, 1.4 ·····.

The ϕ_2=45° sections of corresponding ODF except for as-deformed states are shown in Fig.3 along with the predicted ODF's by the double K-S relation using Eqs. (1) to (3). At 800 ˚C on heating, major components lie around {100}<510>, {110}<211>, {111}<211>. Then after the first transformation, they change to those around {100}<120>, {110}<110>, {221}<102>, etc., and finally a similar ODF to the one at 800 ˚C on heating reappears as seen in Figs. 3 (a) to (c), exhibiting that the texture memory certainly exists in the present experiment.
Even more interesting is that although the recrystallized texture is seemingly reproduced after two transformations, this reproduction or the phenomenon of texture memory is not what this word literally means but only a change into a similar (but different) state of texture. As indicated by arrows in Figs. 3 (a) and (c), the component around ϕ_1=150°, Φ=40° and ϕ_2=45°, which exists at 800 ˚C on heating, is seen to be missing in the final texture. Similar absence of texture components in the final texture has been seen in the other sections of ODF. The predicted textures for the ones after the first and second transformations are shown in Figs. 3(d) and (e) respectively; the values of ω for the first and second transformations are 0.9 and 2.5 respectively. They are calculated from the experimental recrystallized texture in Fig. 3(a); note that for the final texture in Fig. 3(e), transformation calculation was applied to the predicted texture in Fig. 3(d). By comparing with the experimental textures, it is evident that the prediction by the double K-S relation is capable of quantitatively reproducing the texture change during $\alpha \rightarrow \gamma \rightarrow \alpha$ transformation in the ECAP iron, as has been observed in hot-rolled steel and cold-rolled iron [3]. Almost every detail in the experimental texture is observed in the predicted ones including the absence of texture components around ϕ_1=150°, Φ=40° and ϕ_2=45° in the final texture, although slight difference is seen in peak intensity.

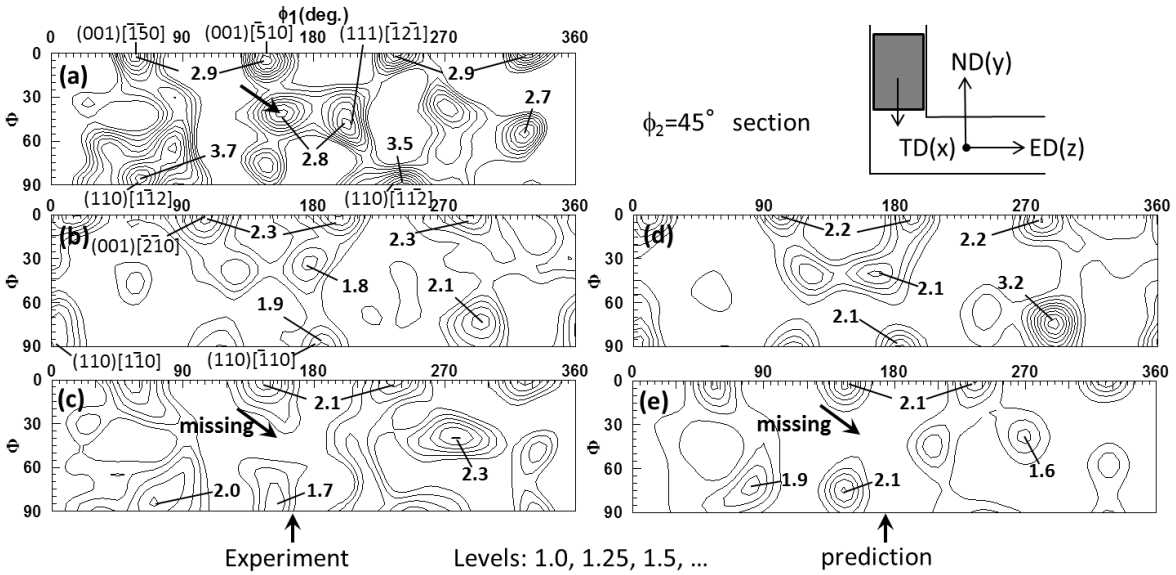

Fig.3 (a to c) Experimental and (d and e) predicted ϕ_2=45° sections of ODF (a) at 800 °C on heating for α, (b and d) at 950 °C for γ and (c and e) at 800 °C on cooling for α.

Therefore, the present analysis of the texture change during the successive transformations in ECAP-processed pure iron indicates that the double K-S relation should indeed be the governing variant selection rule on the phase transformation between α and γ in iron and steel. Finally in Fig. 4 are presented the predicted {111} pole figures corresponding to the Figs.3 (d) and (e), in which a good agreement with the experimental pole figures is seen.

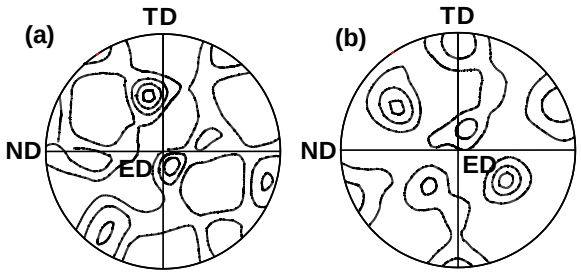

Fig. 4 Predicted (111) pole figures of ECAP-processed iron for (a) γ after heating to 950 ˚C and (b) α after cooling to 800 ˚C. Levels are 1.0, 1.2, 1.4 ·····.

4. Conclusions

As presented above, it is most likely that the mechanism governing the variant selection on phase transformation between α and γ in iron and steel should be the one described by the double K-S relation. Therefore, interphase boundary structures and interfacial energy seem to be the most influencing factor to determine the active variants on such transformation.

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