Proposal of Simplified Modified Williamson-Hall Equation

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Williamson-Hall (WH) plots are characterized by irregular arrangement of data due to the elastic anisotropy in each [hkl] plane. In order to correct the effect of elastic anisotropy, Ungár developed a unique methodology using the contrast factor C, so called the modified Williamson-Hall (mWH) method. When X-ray with the wave length \( \lambda \) was used for diffraction analysis and diffraction angle \( \theta \) and integral breadth \( \beta \) was obtained in each diffraction peak, the following mWH equation is constructed as functions of the parameter \( K = (2\sin \theta \lambda) \) and \( \Delta K = (\beta \cos \theta \lambda) \).

\[
\Delta K = \alpha + \varphi K \sqrt{C + O^2 C}
\]

Here, the parameter \( \alpha \) is dependent on the crystallite size. The parameter \( \varphi \) and \( O \) are constants but the \( O \)-value is much smaller than the \( \varphi \)-value. In the mWH plots in 60% cold rolled ferrite (Fe-0.0056%C), ultra low carbon martensite (Fe-18%Ni) and 20% cold rolled austenite (SUS316L), it was confirmed that the value of \( O^2 C \) is negligibly small. As a result, the following simplified equation is applicable for the analysis by mWH method.

\[
\Delta K = \alpha + \varphi K \sqrt{C}
\]

KEY WORDS: modified Williamson-Hall equation; simplified modified Williamson-Hall equation; elastic anisotropy; ferritic steel; ultra low carbon martensitic steel; austenitic steel.

1. Introduction

In general, radiation diffraction analysis is applied for highly dislocated materials to evaluate dislocation characterization. Williamson proposed a basic approach to evaluate the micro-strain \( \varepsilon \) which is produced by dislocations. When X-ray with the wave length \( \lambda \) was used for diffraction analysis and diffraction angle \( \theta \) and integral breadth \( \beta \) was obtained in each diffraction peak, the following Williamson-Hall (WH) equation is constructed as functions of the parameter \( K = (2\sin \theta \lambda) \) and \( \Delta K = (\beta \cos \theta \lambda) \).

\[
\Delta K = \alpha + \varepsilon K \] 

In this study, full width at half maximum (FWHM) is used instead of integral breadth as with some researchers.2)

Here, the parameter \( \alpha \) is dependent on the crystallite size. Various values are obtained in several diffraction peaks, thus the values of parameter \( \alpha \) and \( \varepsilon \) are determined in the relation between \( K \) and \( \Delta K \). However, linear relation is not obtained usually due to the elastic anisotropy in each [hkl] crystal plane. Such an elastic anisotropy is usually discussed in connection with the orientation parameter \( \Gamma \) which is expressed by the following equation as a function of Miller index {hkl}.

\[
\Gamma = \left( h^2 k^2 + k^2 l^2 + l^2 h^2 \right) / h^2 + k^2 + l^2 \] 

\[ 0 \leq \Gamma \leq 1/3 \] 

Ungár proposed a method to correct the elastic anisotropy in WH plots by the contrast factor \( C \) which is given by the following equation,3)

\[
C = C_{h00} \left( 1 - q \Gamma \right) \] 

where \( C_{h00} \) is the contrast factor in the crystal plane {h00} and \( q \) is a constant, which depend on the screw component of dislocation \( S \) \( (0 \leq S \leq 1) \) as follows.

\[
C_{h00} = (1 - S) C^{E^0} + SC^{S^5} \] 

\[
q = (1 - S) q^E + Sq^S \] 

\( C^{E^0} \) and \( C^{S^5} \) are the contrast factor of edge dislocation and screw dislocation, \( q^E \) and \( q^S \) are the \( q \)-value of edge dislocation and screw dislocation, respectively. They are material constants which depend on the elastic constants: \( C^{E^0} = 0.259 \), \( C^{S^5} = 0.295 \), \( q^E = 2.67 \) in bcc iron and \( C^{E^0} = 0.291 \), \( q^S = 2.32 \) in fcc iron.3) Therefore, once a certain value is given for the parameter \( S \), the contrast factor \( C \) in Eq. (3) is identically determined.

Ungár reconstructed the WH equation as follows applying the contrast factor \( C \), so called modified Williamson-Hall (mWH) equation and the plots of \( \Delta K \) vs. \( K \sqrt{C} \) are called mWH plots.

\[
\Delta K = \alpha + \varphi K \sqrt{C + O^2 C} \] 

Here, \( \varphi \) and \( O \) are the coefficients depending on the micro-structural factors. In the mWH method, the \( C \)-value is determined to minimize the fitting error of mWH plots against Eq. (6) and then the value of parameter \( S \) is introduced from the determined \( C \)-value.

The optimal \( C \)-value is obtained in the plots of \( \Delta K \) vs. \( K \sqrt{C} \) but the analyzing accuracy is greatly heightened adding the value of parameter \( \alpha \). In order to correct the elastic anisotropy in WH plots, authors have developed a new method, so called the direct-fitting (DF) method. Applying the DF method to WH plots, the elastic anisotropy of each crystal plane has been accurately corrected and linear relation is realized. Thus, the \( \alpha \)-value is precisely determined from the fitting line.

In this paper, the \( \alpha \)-value obtained by the DF method was applied to the mWH method using Eq. (6) and then the coefficient \( \varphi \) and \( O \) were obtained in different type of steels; 60% cold rolled ferrite (Fe-0.0056%C), ultra low carbon martensite (Fe-18%Ni) and 20% cold rolled austenite (SUS316L). If the parameter \( O \) is much smaller than \( \varphi \) in every steel, the following simplified equation may be applicable in the analysis by mWH method.
\[ \Delta K = \alpha + \phi K \sqrt{C} \] .......................... (7)

2. Determination of \( \alpha \)-value by the Direct-fitting Method

Figure 1 shows the WH plots in 60% cold rolled ferrite, as an example. The data of \{220\} is not plotted here because the diffraction intensity was weak. The original plots (solid circles) are characterized by irregular arrangement of data due to the elastic anisotropy in each crystal plane. In the DF method, such an elastic anisotropy is corrected by the parameter \( \omega \) which is identified by the ratio of diffraction Young’s modulus; \( \omega = \frac{E_{\text{diff}}}{E_0} \). Here, \( E_{\text{diff}} \) and \( E_0 \) are the diffraction Young’s modulus in each \{hkl\} plane and the standard Young’s modulus respectively. The value of \( \omega \) is identically determined to minimize the fitting error of \( \Delta K \) vs. \( (K/\omega) \) against linear relation. We confirmed that the \( \omega \) value obtained by DF method is almost the same as that calculated by Kröner model. This indicates the reasonability of DF method on the correction of anisotropy in WH plot. The corrected data are plotted by open squares. In the case of bcc iron, the \( E_{\text{diff}} \)-value of \{110\} and \{211\} plane is very close to \( E_0 \) so that the effect of correction is small, while it is found that the elastic anisotropy in the other crystal planes has been accurately corrected by the DF method. The slope gives the \( \varphi \)-value in Eq. (1) and the \( \alpha \)-value is given by the star mark (0.00158 nm\(^{-1}\)). Authors have confirmed that the \( \alpha \)-value can be accurately determined in austenite (fcc iron) by the DF method.

3. Application of the Parameter \( \alpha \) to the Modified Williamson-Hall Equation

As mentioned above, the reliability of parameter \( \alpha \) is so high that it can be fixed in Eq. (6). On the other hand, the relation between \( \Delta K \) and \( K \sqrt{C} \) is changeable depending on the value of parameter \( S \) which governs the \( C \)-value. Therefore, the \( S \)-value was determined to give the best fitting against Eq. (6). Firstly, the result in 60% cold rolled ferrite is shown in Fig. 2. In this case, the best fitting was realized at \( S = 0.260 \). It is found that the \( O \)-value is much smaller than \( \varphi \)-value. Figure 3 shows the cases of ultra low carbon martensite (a) and 20% cold rolled austenite (b). The best fitting was realized at \( S = 0.850 \) in the former and \( S = 0.486 \) in the latter. It is also confirmed that the \( O \)-value is much smaller than \( \varphi \)-value. These results indicate that the right third term in Eq. (6) can be neglected and the simplified equation; Eq. (7) can be applicable for the mWH method.

Finally, Fig. 4 shows the comparison as to the values of parameter \( \varphi \), which were obtained by the quadratic fitting against Eq. (6) (\( \varphi_2 \)) and the linear fitting against Eq. (7)
(ψ1). Regarding ferrite and austenite, several data are added to check the correlation between ψ1 and ψ2. It is found that almost same values are obtained in both fitting methods (ψ1 = ψ2). It should be noted here that negative values are obtained for the parameter $O$ in the case; $ψ2 > ψ1$, although the $O$-value should be positive. In such a case, the $ψ$-value tends to be overestimated. As a result, it is recommended to apply the simplified Eq. (7) is used for the analysis by mWH method. Authors have confirmed that similar result is obtained for the other metals; nickel, copper and aluminum.

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