Image Quality Analysis: A New Method of Characterizing Microstructures

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Polycrystalline aggregates are comprised of three microstructural features: grain centers, grain boundaries, and regions affected by grain boundaries. It is these features that determine the mechanical properties, and any advanced understanding of microstructure–property relations requires their quantitative description. Traditionally, descriptions of microstructures have been based on visualization, i.e., how grains appear in the optical or scanning electron microscope (SEM). While this may lead to classification systems that permit differentiation, it does not allow for quantification, especially in complex microstructures, and does not lend itself to either developing or applying structure–property relationships. The goal of this paper is to present a new approach to the characterization of complex microstructures, especially those found in advanced modern high strength steels. For such steels, the new approach employs the fact that different types of ferrite formed at different transformation temperatures have different dislocation or sub-grain boundary densities. Hence, measuring the degree of lattice imperfection of the grain centers of the ferrite is one way of first identifying, then grouping, and finally quantifying, the different types or forms of ferrite. The index chosen in this study to distinguish the degree of lattice imperfection is the image quality (IQ). Finally, as part of the new approach a procedure has been developed to improve the accuracy of applying IQ measurements.

KEY WORDS: image quality; diffraction pattern; EBSD; microstructure; ferrite; grain boundary; phase identification; lattice imperfection.

1. Introduction

Polycrystalline aggregates are comprised of three microstructural features: grain centers, grain boundaries, and regions affected by grain boundaries. In advanced high strength steels, this picture is further complicated by the possibility of grains being of different phases, and of grains of the same phases but with different degrees of lattice imperfection, i.e., dislocation density or sub-grain boundary density. It is these features that determine the mechanical properties, and any advanced understanding of microstructure–property relations requires their quantitative description. Traditionally, descriptions of microstructures have been based on visualization, i.e., how grains appear in the optical and scanning electron microscope (SEM). This approach led to the well-known Dubé classification1,2 of various types of ferrite grains, based solely on the appearance of these grains. While this classification system does permit differentiation, at least in simple systems, it does not allow for quantification. Hence, the traditional approach does not lend itself to either developing or applying accurate, valid structure–property relationships, which would be applicable to both simple and complex microstructures.

Recent research has shown that modern, microalloyed HSLA steel hot-band coils with yield strengths of 490 MPa contain mixtures of polygonal, non-polygonal, acicular and bainitic ferrite, where the various degree of mixture depends on the thermomechanical processing route.3 While these types of ferrite are somewhat discernable using optical microscopy or SEM, it has not been possible to properly and accurately quantify the relative amount of each type of ferrite using standard image analysis systems.

The EBSD technique has been widely used in analyzing steel microstructures. The typical applications of EBSD include grain/sub-grain size measurements, texture analysis, boundary characteristics, grain orientation and phase identification. All of these applications are based upon the crystallographic orientation map, crystallographic structure differences or lattice perfection differences. However, the complexities of steel microstructures greatly challenge the success of these applications. For some complicated steel microstructures, e.g., mixtures of various types of ferrite in HSLA steels and the microstructure of multiphase steels, the phase or microconstituent identification and quantification is still a major problem confronting many metallurgists. In some recent studies,4,9 the diffraction pattern quality (PQ), also called image quality (IQ), analysis has been noted and used to investigate recrystallization behavior and phase transformations. However, only limited studies have been conducted dealing with the effects of the experimental factors and the data processing algorithms on the accuracy of IQ analysis results. Although some valuable information has been gained and interesting results have been published,
there are still large amounts of information being ignored or neglected during the over-simplified data processing. For example, IQ values not corrected for the grain boundary contribution will be misleading, possibly causing investigators to incorrectly determine the level of the IQ or its volume fraction.

In this paper we present a new approach to the characterization of complex microstructures such as may be found in high strength steels. The new approach is based on the fact that the different types of ferrite produced at different temperatures during cooling, for example following hot rolling, will have different densities of dislocations or sub-grain boundaries. In other words, measurement of the lattice imperfection at the grain centers is one way of first identifying, then grouping, and finally quantifying, the different types of ferrite. The index chosen to distinguish the degree of lattice imperfection is the image quality (IQ); a lattice distorted by crystalline defects such as dislocations and sub-grain boundaries will have a distorted Kikuchi Pattern, leading to a lower IQ value. It can also be noted that because nanohardness increases with lattice imperfection, we expect there to be an inverse relationship between IQ and micro- and/or nanohardness.

This new approach of using IQ to characterize microstructures is particularly interesting because it provides a means of quantifying the amounts of various types of ferrite in complex HSLA steel microstructures. Depending upon the transformation behavior during cooling, it is not uncommon for the polygonal, non-polygonal, acicular and bainitic forms of ferrite to co-exist in one sample, especially in HSLA steels with yield strengths over 350 MPa. These different types of ferrite are often readily discernable in optical microscopy and SEM. However, measuring their volume fractions is not easily accomplished using conventional quantitative metallographic techniques. Since both the types of ferrite and the IQ level of the individual ferrite grains vary with dislocation density, the measurement of the spectrum of IQ values in a given samples is necessary.

To take full advantage of the new IQ approach, the effects of image processing on the IQ values are minimized through a normalization procedure; a model considering the effects of grain boundaries on the IQ distribution curve is developed; and a multi-peak model for analyzing multi-component microstructures is introduced. These techniques and some example applications will be discussed in this paper.

The analysis of the IQ spectrum is a powerful and unique way of quantifying complex microstructures in HSLA steels, and is critically important to understanding the origins of strength in HSLA steels.

2. Experimental Procedure

2.1. Materials and Processing

Three steels were examined in this study and their chemical composition is shown in Table 1. Steel A is an IF steel. Starting with commercial hot band, Steel A was cold rolled to a reduction of 50%. Afterwards, two samples were normalized by reheating to and holding at 950°C for 30 and 90 s, respectively, followed by air cooling to room temperature. The resulting microstructures are designated A0 and A1, and although both have a homogeneous, polygonal ferrite structure, the grain size is different. With the A1 condition, two different amounts of cold deformation, 15% and 25%, were applied to develop microstructures A2 and A3, respectively. A2 and A3 are basically polygonal ferrite as well, but having been deformed, they contain different dislocation densities.

Steel B is a dual phase steel. Starting with commercial hot band, Steel B was reheated and held at 806°C for 90 s and water quenched to develop a martensite+polygonal ferrite microstructure, which is identified as B0.

Steel C is HSLA steel. Laboratory simulated hot-rolling was carried out with the commercial as-cast slab material. The samples were reheated to 1200°C for 30 min, air cooled to 1150°C and rolled in three passes of 50% each, and finished at 900°C. From 900°C, the sample was water-spray cooled to 550°C and then furnace cooled to room temperature for simulation of the cooling stage of the strip processing. The microstructure C0, developed from this procedure, is a typical HSLA steel hot band microstructure with various types of ferrite and some carbon rich microconstituents.

A summary of the microstructures developed is given in Table 2.

2.2. Orientation Imaging Microscopy (OIM) Parameters

The EBSD data were collected using the TSL OIM Data Collection Software with the Philips XL-30 FEG SEM system. The standard operational procedure of EBSD observation was employed, with 15 kV voltage and a spot size of 4 (corresponding to a beam diameter in the order of 50 nm) were applied. The frame number was always set at 8 and the hexagonal scan mode was used with step sizes of 2 µm and 0.5 µm. The choice of step size used in data collection can also affect the accuracy of the results, especially when the grain and sub-grain boundaries are of interest. It has been shown that to obtain an accuracy of 10%, at least 5 pixels per grain are required, and for an accuracy of 5%, a minimum of approximately 8 pixels per grain are required. Since the grain sizes of the microstructures of Steels A and B have been estimated to be larger than

| Material Code | Al   | P    | C    | Mn   | Si  | N   | Nb  | Ti  | V   |
|---------------|------|------|------|------|-----|-----|-----|-----|-----|
| A             | 0.041| 0.009| 0.002| 0.15 | 0.007| 0.0027| 0.021| 0.036| -   |
| B             | 1.09 | 0.013| 0.15 | 1.55 | 0.006| 0.003| -   | -   | -   |
| C             | 0.045| -    | 0.078| 3.3  | 0.0032| 0.0043| 0.038| 0.05 | -   |

| Microstructure Code | Microstructure               |
|---------------------|------------------------------|
| A0                  | Polygonal ferrite with small grain size |
| A1                  | Polygonal ferrite with large grain size |
| A2                  | A1 + 15% cold deformation    |
| A3                  | A1 + 25% cold deformation    |
| B0                  | Martensite + Polygonal ferrite |
| C0                  | Mixture of different types of ferrite |
20 µm, the step size of 2 µm was acceptable for these two series. The step size of 0.5 µm was employed for C0 microstructure, which has a finer grain size. By choosing different step sizes for different grain sizes, the error is reduced significantly.

2.3. Data Analysis

The general analysis of the EBSD data was conducted by using the commercial TSL OIM Analysis software. A gray scale image-quality map of a polygonal ferrite microstructure developed by using this software is illustrated in Fig. 1. As clearly seen in this figure, the lower image quality is in the darker areas adjacent to the grain boundaries. In these grain boundary regions (GBR) the low image quality is due to the interference of diffraction patterns from two grains having different orientations. This explanation has been widely accepted. However, the effects of the GBR on the analysis of the IQ spectrum have not been previously considered and their importance has been neglected.

To better interpret an IQ spectrum, a newly developed procedure will address three main tasks: (i) the contribution of the GBR, (ii) the normalization of IQ values and (iii) the statistical distribution.

2.3.1. Accounting for the Grain Boundary Region (GBR) Contribution

In this work, the grain boundary is defined by the misorientation of the two neighboring scanning points. In the commercial TSL software, the statistical information on grain boundary misorientation can be calculated; however, there is no means of identifying or studying the properties of any special grain boundaries of interest. In other words, it is impossible to filter out the GBR pixels. To mark out the GBR scan points, a technique was developed. In this technique, the misorientation between every two neighboring scan points is calculated based on its definition as described by Randle. The grain boundary is defined as any interface with a misorientation larger than 15 deg. The GBR covers the scan points that are contiguous with the grain boundaries, as illustrated in Fig. 2. After examining all the scan points, the GBR points can be marked for further analysis.

2.3.2. Normalizing IQ Values

The most important hurdle to the application of image quality in phase identification is the fact that the IQ value is very sensitive to many operating factors, including the image processing conditions. These factors may confuse the analysis of the information from the microstructure itself and significantly reduce the ability to compare different sets of IQ values. Normalization of IQ values is a way to minimize these misleading effects.

Assuming that the operating factors have an equal effect on each constituent in the microstructure, it is the absolute image quality values, not the relative image quality values from constituent to constituent, that are really influenced by the operating conditions. The normalized IQ value can be calculated as.

\[ \text{IQ}_{\text{Normalized}} = \frac{\text{IQ}_{\text{Initial}}}{\text{IQ}_{\text{Standard}}} \times 100 \]  \hspace{2cm} \text{(1)}

where IQ_{Initial} is the absolute IQ value gained directly from experiment; and IQ_{Standard} is the average IQ value of a standard sample, which is presumed to have a perfect crystal structure and to therefore give the highest IQ value under the same EBSD processing conditions.

Equation (1) can be used to normalize various kinds of microstructures with extremely different components, because they are normalized according to an independent IQ_{Standard}. To compare microstructures with the same components but different volume fractions thereof, a simplified equation, Eq. (2), can be used. The us of Eq. (2) does not need the information of the standard specimen and therefore saves time in scanning.

\[ \text{IQ}_{\text{Normalized}} = \frac{\text{IQ}_{\text{Initial}} - \text{IQ}_{\text{Min}}}{\text{IQ}_{\text{Max}} - \text{IQ}_{\text{Min}}} \times 100 \]  \hspace{2cm} \text{(2)}

![Fig. 1. A gray scale image-quality map of the fully recrystallized polygonal ferrite microstructure.](image)

![Fig. 2. Schematic of the Grain Boundary Region (GBR). Each cell represents a scan point; the heavy black lines are the grain boundaries and the adjacent cells in dark gray are GBR points.](image)
where $IQ_{\text{Max}}$ and $IQ_{\text{Min}}$ are, respectively, the maximum and the minimum IQ values in the scanning set.

In this study, the comparison of Steel A microstructures has been conducted using Eq. (2) for normalization.

2.3.3. Normal Distribution and Multi-peak Model

Typically, the profile of the IQ distribution is bell-shaped, \(^{12}\) our results will confirm later. If we assume a normal distribution, then for a single microconstituent a mean and standard deviation can be assigned to the IQ distribution of a single symmetric peak of the distribution curve. Whenever an asymmetric shaped distribution curve is observed, it implies that more than one microconstituent of different mean IQ values exists. The multi-peak model is developed on this assumption and used to divide the whole distribution curve into several normal distributions, each of which represents a certain microconstituent.

The multi-peak model can be described as:

\[ N = \sum_{j=1}^{k} n_i \]  
\[ IQ = \sum_{j=1}^{k} ND(n_i, \mu_i, \sigma_i) \]  
\[ \text{Min}(k) \]  
\[ |IQ - \sum_{j=1}^{k} ND(n_i, \mu_i, \sigma_i)| \leq \varepsilon \]

where $N$ is the number of the total scan points in the file; $k$ is the number of normal distributions in the simulation; $\varepsilon$ is the minimum acceptable error; $ND(n_i, \mu_i, \sigma_i)$ is the $i$th normal distribution with the total data number of $n_i$, the group mean value of $\mu_i$ and the standard deviation of $\sigma_i$. Adjusting every normal distribution and satisfying the Eqs. (3)–(5) produces a minimum difference between the initial IQ distribution and the sum of all single normal distributions, as shown in the Equation (6). In this procedure each of these normal distributions represents one component in the microstructure.

2.4. Metallurgical Interpretation of Image Quality

The IQ is proportional to the sharpness of the Kikuchi Pattern, which is related to the presence of crystalline defects. An elastically distorted lattice will have a smeared Kikuchi Pattern and a low IQ. A highly dislocated lattice will be expected to have a low IQ and a high nanohardness. To test this hypothesis, nanohardness measurements were taken on pre-selected areas of known IQ using the Nanoindentor equipment at the Oak Ridge National Laboratory (ORNL). In addition, microhardness measurements were conducted in the grain centers of different IQ values.

3. Results and Discussion

3.1. Grain Boundary Region

The gray scale IQ maps of microstructures A0 and A1 are shown in Fig. 3. It is not surprising to find that the darker areas, which indicate lower image quality, are especially located in the vicinities of grain boundary. When the GBR is included, as shown in Fig. 4(a), for both A0 and A1 microstructures, there are two distinguishable peaks in the IQ distribution curve. Since there is only one simple microconstituent in both microstructures, the lower IQ peak could only correspond to the GBR points. With a smaller grain size, A0, there is a higher area fraction of grain boundary
per unit volume than with the larger grain size of A1. This higher fraction of grain boundaries implies a larger low-IQ peak, which is in fact observed in the IQ distribution curve of A0. After filtering out the GBR points with the algorithm mentioned earlier, two symmetric IQ distribution curves for both microstructures are achieved, as shown in Fig. 4(b). This confirms that the lower IQ GBR points are the only source of the peak observed in the low IQ range and for a microstructure with a single microconstituent, the IQ distribution is symmetric.

The GBR could also affect the mean IQ value of each peak in the distribution curve. As seen in Eq. (2), IQ_{Min} and IQ_{Max} are normalized to be 0 and 100, respectively. For a certain absolute IQ distribution, IQ_{Min} and IQ_{Max} values would affect the mean IQ value of the peaks after normalization. For the A0 and A1 microstructures, the IQ_{Min} value most likely comes from the low IQ GBR peak. For unknown reasons, the IQ values of the GBR usually have a large variation. This makes the normalized IQ distribution less predictable. Under the effects of the GBR, the peak positions of the two distributions, Fig. 4(a), are not well matched. Whereas with GBR filtered out, Fig. 4(b), the mean IQ values are approximately the same.

### 3.2. Strain Distribution

There are two main purposes of this part of study. One is to confirm that the image quality is directly related to the lattice imperfection (dislocation density and/or defect density); the other one is to quantify the retained cold strain using IQ analysis, based on the symmetric distribution of the single phase and multi-peak model.

The image quality maps of microstructures A2 and A3 strained 15 and 25%, respectively, are shown in Fig. 5. The areas in gray have normalized IQ value lower than 60 and the areas in white have IQ values higher than 60.

Fig. 5. IQ maps of (a) A2 microstructure and (b) A3 microstructure. Areas in gray have normalized IQ value lower than 60 and the areas in white have IQ values higher than 60.

In the initial microstructure, the difference of the low-angle misorientation distribution in these two microstructures could only arise from the different amounts of applied cold deformation. An apparent correlation between the high dislocation densities introduced by cold deformation and the low image quality is evident. Based on this finding, the distribution of the retained strain can be examined. As shown in Fig. 5, the strain distribution indicated by the low IQ areas is inhomogeneous. When the strain is relatively small, Fig. 5(a), there are very few low-angle misorientation boundaries found inside the grains. This suggests that the applied strain was accommodated by grain boundary sliding or by reverse shear inside grains. With increasing strain, as in Fig. 5(b), the low IQ area extended into some grain centers. The selection of grains where strain is retained, which is directly related to the yielding behavior of steels, might be determined by the orientation of the grains. A more detailed treatment of this topic deserves to be undertaken elsewhere.

The multi-peak model has been used to analyze the cold deformed A2 and A3 microstructures, and the results are shown in Fig. 7. The initial EBSD data have been normalized and the grain boundary contributions have been filtered. For both microstructures, the IQ distribution curve could be best fitted with two normal distribution curves. The low IQ peak corresponds to the areas with retained strain; while the high IQ peak represents those areas that are affected very little by the deformation. The fraction of the data points of each peak is given in Table 3. It is somewhat surprisingly that the fraction of the low IQ peak numerically matches very well with the strain applied. However, this result does appear to support the idea that the IQ analysis and the multi-peak model can be used to identify the strain-retained area and quantify the amount of cold deformation. Further work is in progress to decide whether this good agreement is real or fortuitous.
3.3. Measurement of the Volume Fraction of Martensite

As one simple application of IQ analysis, the martensite volume fraction has been measured for the dual phase steel with the $\alpha/\alpha'$ microstructure, B0, and the results are shown in Figs. 8 to 10.

An optical micrograph of the B0 structure in Fig. 8 shows the mixture of polygonal ferrite and martensite. As expected from the difference in dislocation density of these two phases, two distinct image quality regions are observed in the IQ map of Fig. 9, with polygonal ferrite being the light area with high IQ and martensite being the dark area with low IQ.

Further analysis of the normalized IQ data was conducted using the multi-peak model. As shown in Fig. 10, two normal distribution peaks have been constructed and their sum perfectly matches with the distribution curve of the experimental data. Assuming all data points in the low image quality peak come from martensite, the fraction of the low IQ peak gives the volume fraction of the martensite phase in this mixed-phase microstructure, which is found to be 43.9%. Compared to the manual measurement from optical

| Microstructure Code | Low IQ Peak Fraction | High IQ Peak Fraction | Cold Strain |
|---------------------|----------------------|-----------------------|-------------|
| A2                  | 0.17                 | 0.83                  | 0.15        |
| A3                  | 0.27                 | 0.73                  | 0.25        |
microscopy, which is approximately 40%, the martensite volume fraction estimated using IQ analysis is reasonably accurate.

The major advantage of adopting the multi-peak model for IQ analysis is that it can be applied to various kinds of asymmetric IQ distribution curve. IQ analysis has been used in the past to measure martensite volume fractions in $\alpha + \alpha'$ microstructures only in the case of double peaks detected.\(^6\) In the current work, the new multi-peak model does not require any threshold to be pre-selected. Furthermore, the capability of this technique has been enhanced by considering the grain boundary influence and dealing with the condition when no trough exists in the distribution curve.

The accuracy of the IQ analysis can be affected when areas of unexpected high dislocation density areas are developed. For the B0 microstructure, during the martensitic transformation upon quenching, a significant number of dislocations are produced in the ferrite grains surrounding the martensite. The image quality of these ferrite areas is much reduced and they might be mistaken for martensite. This explains why the measurement using the IQ technique is slightly higher than the one gained from traditional optical or SEM methods. An effort to minimize and correct this error is ongoing.

3.4. Analysis of a Multi-phase (Mixture of Types of Ferrite) Microstructure

IQ analysis and the multi-peak model have been adopted to analyze the C0 microstructure, a mixture of several different austenite decomposition products as the optical micrograph shows in Fig. 11. The corresponding IQ analysis results are presented in Figs. 12 and 13. Because various cooling rates were used in the run-out-table simulation, i.e., air cooling and water spray cooling, followed by coiling, taken together with the complex CCT diagram expected for this steel, several types of ferrite were formed at different temperatures during cooling. For a complex microstructure like C0, the visual identification of the ferrite types based on the morphological differences is extremely difficult, if not impossible. It is therefore nearly impossible to get an accurate measure of the volume fraction of the austenite decomposition products by using any of the traditional microstructural analyses.

EBSD maps of the C0 microstructure are shown in Fig. 12, in which (a) is the grain boundary and subgrain boundary map and (b) is the gray scale image quality map. It is observed that the grains with interior subgrain boundaries always have relatively lower IQ values compared to those without subgrains. The ferrite types formed at low temperatures, e.g., acicular and bainitic, have a higher degree of lattice distortion and a larger density of subgrain boundaries. Even for the grains without subgrain boundaries, the IQ values vary noticeably from one grain to another. This variation of IQ values implies a difference in lattice imperfection, e.g., dislocation density, which is very much determined by the mechanism and temperature of formation of the ferrite type. Consequently, the differentiation of IQ val-
ues caused by the lattice imperfection serves to identify the different types of ferrite.

The result of applying the multi-peak model to the C0 microstructure is shown in Fig. 13. A total of five normal distribution peaks are summed up and the difference from the experimental data curve is around 1.7%. Because the traditional classification of ferrite is mainly based on the visualized grain morphology and the IQ method relies on the lattice imperfection, the correspondence of the multi-peaks in Fig. 13 to the particular ferrite types can only be assumed at present. The first assumption is that each component of the final microstructure has its own, individual characteristic peak in the IQ distribution curve. The second assumption is that the mean value for each IQ peak decreases with the falling transformation temperature of each type ferrite. Thus, some correspondence of the microstructural variation and the IQ distribution curve may be possible, as indicated in Fig. 13.

The IQ analysis itself is a new method of characterizing microstructures since it is based on a 3-D view of lattice imperfection, as opposed to the traditional analysis based on 2-D surface visualization. Furthermore, the potential application of this technique has been greatly expanded since the IQ value shown in Fig. 14 to be inversely proportional to the mechanical properties as represented by the microhardness or nanohardness. This result is not surprising, given that the lattice defects influence both the IQ and mechanical properties, but it does raise the promise that the IQ approach will become a valuable tool in developing microstructure-mechanical property models of complex modern high strength steels.

4. Conclusions

To characterize complex multi-component microstructures in a more effective and detailed fashion, a new procedure using EBSD diffraction pattern image quality has been developed. In this procedure, the variation of IQ values caused by image processing has been minimized through a normalization procedure. Also, for the first time, the influence of the GBR on the image quality distribution is accounted for when characterizing microstructures. Finally, a multi-peak model simplifies the task of separating the IQ spectrum into component peaks and thereby strongly enhances the capability of the IQ procedure to analyze more complicated microstructures.

Using this innovative IQ procedure, dislocation density gradients in cold deformed samples have been successfully observed. This development, combined with the proper treatment of the grain boundary effects, may be used to study the recrystallization behavior with improved accuracy. There is also the expectation that when combined with the EBSD orientation map, the IQ procedure will become a useful tool for studying fundamental deformation mechanisms.

In another illustrative application of this technique, the martensite volume fraction was evaluated in a martensite+ferrite microstructure. However, the observation of high
dislocation density areas in the ferrite grains adjacent to the martensite is a previously unacknowledged source of error, even though it sheds light on the inhomogeneous nature of the retained strain.

Finally, this new IQ procedure may be used to analyze and quantify the complex microstructures of HSLA steels with yield strengths over 350 MPa and which contain different types of ferrite. This application may be especially valuable for relating microstructure to mechanical properties, as suggested by the demonstration that the IQ values are inversely related to the nano- and micro-hardness.

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