X-ray Fourier Analysis on Rolling Contact Fatigue Layer Formed in Rail

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The crystallite size and dislocation density in RCF (rolling contact fatigue) affected layers have been identified using X-ray Fourier analyses on serviced rails. The evaluation of the crystallite size and dislocation density is based on modified Williamson-Hall and Warren-Averbach models. This evaluation enables quantification of the microstructure evolution in the RCF layer with the increase of accumulated loading (in terms of MGT – Million Gross Tonnes) as well as the identification of the most deteriorated locations in the RCF layer. In summary, the surface layer experiences the highest deterioration in the evaluated cases.

Keywords: rail, rolling contact fatigue, X-ray Fourier analysis, crystallite size, dislocation density

1. Introduction

The repetitive contact of a wheel on a rail forms a RCF (rolling contact fatigue) affected layer on the surface of the rail head. If this RCF on the rail significantly progresses, it can cause rail failures such as squats, headchecks, flaking, etc. which could in turn lead to the potential risk of the rail breaking. Hence, controlling the risk of a rail breaking will help not only improve the running stability and safety of the rolling stock but also increase the service life of the rail with less maintenance cost.

Rail grinding cars have started to artificially remove the RCF affected layers formed in rails and have greatly contributed to suppressing rail failures. In order to make this type of operation effective, several aspects must be considered namely the grinding depth and distance, the interval between operations, the number of available grinding cars and so on. For in-service rails being ground for the first time in particular, it is also necessary to consider the influence of the RCF affected layers already formed. Therefore, we should investigate how to remove the RCF layers so as not to cause rail failures in the practical range. Even in the case of rail replacement, if the degree of RCF formation can be evaluated, rail replacement work would be more efficient.

Many research activities have been devoted to identifying the formation process of the RCF affected layer in a rail from computational and experimental aspects [1 - 4] as it is essential to grasp its formation process to achieve the effective suppression of rail failures. For the experimental approaches to the RCF, optical microscopes, indentation measurement, X-ray crystallography, high magnification microscopes (e.g. SEM, TEM), etc. have been employed. However, the degree of plastic deformation in the contact surface of the RCF layer has not been fully quantified yet. Furthermore, the contact patch between a wheel and a rail is exposed to complex stress conditions such as contact pressure, tangential stress, thermal influence exerted by the wheel, residual stress in the rail and so on. This is the reason why their contribution to the RCF layer formation has not yet been clarified.

This study focuses on the degree of plastic deformation in the RCF affected layer and then a new approach applies the X-ray Fourier Analysis method to identify it. X-ray Fourier analysis enables estimation of the degree of plastic deformation by quantifying the X-ray crystallite size and dislocation density. It has already been employed to reveal the dislocation density and the X-ray crystallite size of ultra-fine grained metals in a severely strained state [5 - 7]. We have applied this method to the quantification of RCF layers formed in serviced rails through the investigation of its applicability.

2. X-ray crystallite size and dislocation density

The X-ray crystallite size is schematically indicated in Fig. 1. It is a grain size defined by X-ray measurement and corresponds to the area where crystal orientation is aligned in the same direction. The dislocation density means the number of crystal defects and is closely related to the plastic strain generated in a material. Figures 2(a)-(c) show the effect of the strain on the X-ray diffracted peak. If the material is not strained, a sharp X-ray diffracted peak is obtained. This X-ray peak position is shifted by the elastic strain and is back to the original position after the material is unloaded. The X-ray peak is broadened if the material is plastically strained. As shown in Fig. 3, the X-ray diffracted peak of a RCF affected rail is broadened with shifting the peak position. The change of the X-ray crys-
tallite size and dislocation density gives influence on the geometry of the X-ray diffracted peak. In other words, the X-ray crystallite size and dislocation density is revealed by evaluating the geometry of X-ray diffracted peaks for the serviced rail with RCF accumulation.

3. Microstructure evolution due to the RCF

Figures 4(a)-(c) show microstructure evolution due to the RCF. Virgin rail steel mostly consists of pearlitic grains. If it is subjected to RCF from the repetitive wheel contact, plastic strain (dislocation) is induced in the grains and/or at the boundary of the grains (see broken lines in Fig. 4(b)). The grains are divided into smaller ones by the piled up dislocation with more induced plastic strain as shown in Figs. 4(b) and (c). Eventually, the changes to the microstructure can be visually identified as plastic flow and the refinement in the microstructure subjected to RCF, which corresponds to the history of RCF accumulation. The quantification of this evolution will reveal the RCF deterioration mechanism of the rail.

4. X-ray Fourier Analysis

X-ray Fourier Analyses were carried out to investigate the degree of plastic deformation in the RCF affected layers of serviced rails by analyzing the X-ray diffracted peak geometry. Williamson et al. proposed an analytic method to distinguish strain and crystallite size contribution to the X-ray peak broadening, which is widely known as the Williamson-Hall equation [8]. It is described as

\[ \Delta K = \alpha \varepsilon + \frac{\alpha}{K} \]  

with expressions of \( K = 2 \sin \theta / \lambda \) and \( \Delta K = 2 \cos \theta (\Delta \theta / \lambda) \), where \( K \), \( \theta \) and \( \lambda \) are the magnitude of diffraction vector, the X-ray diffraction angle and the wave length of the incident X-ray, respectively. \( \varepsilon \) denotes the strain contribution to the peak broadening. \( \alpha \) is described by \( 1/d \) where \( d \) is the X-ray crystallite size as long as the broadening of the X-ray diffracted peak is evaluated by the integral width. Equation (1) gives us both values of the crystallite size and strain through a monotonous function of \( K \). Unfortunately, the steel consisting of Fe has strain anisotropy, which made it hard to analyze using a monotonous function [9]. Ungar et al. adopted a combination of the dislocation contrast factor, \( \tilde{C} \) and the magnitude of diffraction vector, \( K \) as a new scaling factor for suppressing strain anisotropy [5]. On the assumption that dislocation accounts for most of the contribution of the strain to the peak broadening, they proposed a modified Williamson-Hall equation as shown below.

\[ \Delta K = \alpha + \beta \tilde{C}^{1/2} + O(K^2 \tilde{C}) \]  

where \( \tilde{C} \) is the dislocation contrast factor based on the elastic anisotropy constants of Fe. \( \beta \) is a constant relating to the dislocation density and \( O \) indicates non-interpreted higher-order terms. Ungar et al. combined (2) with (3), which is called a modified Warren-Averbach equation, to experimentally estimate the dislocation density. The \( K\tilde{C}^{1/2} \)
value determined in (2) is substituted into (3) given by
\[
\ln A(L) = \gamma - \frac{\rho L^2 \pi b^2}{2} \ln \left( \frac{R_e}{L} \right) K^2 C + P(K^2 C)^2
\]

where \( A(L) \) is the real part of the Fourier coefficient for X-ray peak broadening, determined by adopting the fitting function of the pseudo Voigt function consisting of the Gaussian and Lorentzian functions. \( L \) is defined as the Fourier length. \( \rho, b \) and \( R_e \) indicate the dislocation density, the value of the Burgers vector for Fe \( (b = 0.248 \text{ nm}) \) and the value relating to dislocation, respectively. \( P \) and \( \gamma \) are constants. As long as \( \ln A(L) \) is plotted with \( L \) fixed as a function of \( K^2 C \), the coefficient of the first-order term on the right-hand side of (3) is given. The \( \rho \) value of dislocation density is evaluable through the linear fitting procedure with these coefficients calculated for the various \( L \) values.

5. Experiment

Two kinds of serviced tangent rails with the different accumulated loadings were prepared for this study. The specifications of these rails are shown in Table 1. The place from which small samples were cut out for the X-ray measurement is indicated in Fig. 5. The small samples were taken so that their top surfaces included an area of the running band. Then the small samples were subjected to X-ray measurement. The X-ray measurement was carried out from the top surface downward into the inner part of the sample with repeated electrical polishing to avoid exerting extra stress to the samples. The depth of each electrical polishing was chosen to evaluate the distribution of the X-ray crystallite size and dislocation density in the samples. The output of the X-ray measurement at each depth was analyzed by X-ray Fourier Analysis to estimate the X-ray crystallite size and the dislocation density. As shown in Fig. 6, \( \text{Cu}K\alpha \) radiation was employed as an incident X-ray as the X-ray penetration depth is shallow compared to other incident X-rays such as \( \text{Cr}K\alpha \). As shown in Fig. 6, \( \text{Cu}K\alpha \) is suitable as an incident X-ray because of the measurement of drastic variation in the RCF affected layer. Hence, the shallow X-ray penetration depth of \( \text{Cu}K\alpha \) for each crystal plane available for the X-ray measurement with \( \text{Cu}K\alpha \) is regarded as the six crystal planes of (110), (100), (211), (220), (310) and (111). The X-ray equipment with \( \text{Cu}K\alpha \) as an incident X-ray was operated at angle increments of 0.02° for a duration of 10 sec to measure and detect the diffracted X-ray peak geometry for each crystal plane using the graphite monochromator mounted at the diffraction side of the X-ray goniometer. Then we estimated the proper values of \( C \) and \( a \) on the right hand of (2) through the repetitive fitting procedures after substituting \( a_0 \) calculated on (1) into the first term of the right hand of (2). The dislocation density at each depth was evaluated through the proper value of \( K^2 C \) for each crystal plane on (2). If the coefficient of the second term of the right hand in (3) is regarded as \( \gamma L \), it is transformed as
\[
\frac{Y(L)}{L^2} = \frac{\rho \pi b^2}{2} \left( \ln R_e - \ln L \right)
\]

On (4), the dislocation density, \( \rho \) is experimentally calculable through the fitting procedure for the properly fixed \( L \) values.

6. Results and discussion

Figures 7(a) and (b) show the optical microstructures of the longitudinal sections of the running bands for the serviced tangent rails A and B in Table 1. In the case of rail A, the plastic flow was observed down to the position of about 40 μm in depth from the contact surface. The optical microstructure below a depth of roughly 40 μm did not seem to be less strained than the part above 40 μm. In the plastic flow observed for rail A, the RCF due to repeated wheel contact deteriorated the initial microstructure of the
rail steel, resulting in the enhancement of the microstructure refinement. As mentioned above, microstructure refinement stems from RCF accumulating plastic strain (dislocation) below the contact surface. Furthermore, growth of plastic flow is influenced by tangential stress acting on the contact patch between a wheel and a rail. On the other hand, the white etching layer beneath the contact surface was formed presumably by the thermal influence of the contact with a wheel. The optical microstructure was plastically flown down to the depth of approximately 400 $\mu$m under the white etching layer. Compared with the optical microstructures below the area affected by plastic flow in rails A and B, rail B exhibited more qualitative deterioration as accumulated loading increased, and due to difference of the wheel/rail contact conditions, etc. Hardness measurements are often adopted to evaluate the microstructure change for an experimental approach. However, it is difficult to quantify any drastic variation in the thin layer of less than 50 $\mu$m thick just beneath the contact surface, in the case of rail A. It was noted that as far as it was possible to observe, rail failures such as squats and flaking were not visually confirmable on either rail A or B.

RCF cracks are preferentially initiated in the ferrite grain of the rail steel [10]. Based on this fact, X-ray measurements were an effective method for quantifying RCF as they can evaluate in isolation the ferrite grain with RCF. Hence, X-ray Fourier Analysis was employed with a view to clarifying RCF deterioration in rails. Figures 8(a) and (b) show the results of analyzing the X-ray measurements by (1) and (2) for rails A and B. As shown in Fig. 8(b), (2) can suppress the strain anisotropy on each crystal plane of the rail steel by adopting the quadratic function $K C^{1/2}$ for rail A.

Figure 10 indicates the distribution of the X-ray crystallite size and dislocation density evaluated through the X-ray Fourier Analysis for rails A and B in the depth direction. The plastic strain accumulates in the surface layer of the rail, resulting in a decrease of X-ray crystallite size and an increase in dislocation density. Hence, the left y-axis in Fig. 10 is arranged in reverse to facilitate understanding of RCF deterioration. This indicates that RCF deterioration worsens if the measured position is close to the contact surface as shown by the plotted data. Compared with rail A, rail B tends to exhibit small X-ray crystallite size and large dislocation density, which is consistent with the RCF measurement result.
Fig. 9 Analytic results for the contact surfaces of rails A and B by (3) and (4).

was that the contact surfaces of rails A and B were more deteriorated than any other positions measured deeper below the contact surface. In particular, RCF was drastically less influential below the contact surfaces down to approximately 50 µm deep for rail A and approximately 250 µm deep for rail B and finally the X-ray crystallite size and the dislocation density reached the material levels. It is conceivable that such differences and similarities can be attributed to RCF evolution generating the microstructure refinement, plastic flow and the white etching layer, etc. as shown in Figs. 7(a) and (b). For rail A, the dislocation density increased once in the depth range of around 50 to 250 µm. On the other hand, rail B appeared to plateau in X-ray crystallite size and dislocation density distribution at depths of between 100 to 700 µm around. Considering this fact, it is plausible that the detrimental factor affecting the RCF evolution is different between the surface layer and the sub-surface layer. In other words, the RCF deterioration in the surface layer is mostly derived from the tangential stress acting on the contact patch and the surface roughness contact between a wheel and a rail, and so on, whereas in the sub-surface layer, Hertzian stress due to the wheel/ rail contact is influential on the RCF deterioration. Thus, drastic variation in the microstructure can be analyzed by the X-ray Fourier Analysis, and it is also possible to evaluate the degree of the RCF evolution from the surface into the sub-surface layer by the same analytic method.

7. Summary

We have applied the X-ray Fourier Analysis to identifying the degree of the material deterioration of the RCF affected layer of the serviced rails. The X-ray Fourier Analysis estimates the X-ray crystallite size and dislocation density referring to the degree of plastic deformation. The following are obtained in this study.

CuKα radiation as an incident X-ray is suitable for the in-house experiment to quantify the drastic microstructure variation in the RCF affected surface layer as it has the shallow X-ray penetration depth for rail steel compared with other major X-ray radiation sources resulting in the high depth resolution. The drastic microstructure variation in the RCF affected surface layer of the serviced rails is evaluable through the X-ray Fourier Analysis with the strain anisotropy of steel suppressed. The same analytic method is basically available for the area from on the contact surface down into the sub-surface of the RCF affected layer. The investigation of the serviced rails through the X-ray Fourier Analysis revealed that the distributions of the X-ray crystallite size and the dislocation density evolved in accordance with the microstructure change due to the RCF as well as the increase of the total loadings. Furthermore, the contact surface of the RCF affected layer experienced the highest deterioration in the evaluated cases. The X-ray Fourier Analysis is expected to help compare the degree of the RCF evolution for various serviced rails and clarify the RCF detrimental behavior.
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