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Evaluation of material deterioration of rails subjected to rolling contact fatigue using x-ray diffraction

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ABSTRACT

Crystallite size and dislocation density in RCF (rolling contact fatigue) affected layers have been identified using x-ray measurements for the serviced rails and rail disk sample. The evaluation of crystallite size and dislocation density was based on the modified Williamson-Hall and Warren–Averbach analyses. This evaluation enabled to provide a quantification of the microstructural evolution in the RCF layer with the increase of accumulated loading as well as an identification of the most deteriorated locations in the RCF layer. In summary, the surface layer experienced the highest deterioration in all evaluated cases. Furthermore, the accumulation of loading (in terms of MGT—Million Gross Tonnes) increased the depth of the surface RCF layer. A (111) texture formation was observed in the subsurface RCF layer after some accumulated operational loading. Further conclusions from the study are that it is essential to consider the surface roughness in the contact patch in addition to the microstructural variations such as the refinement, the plastic flow, etc., since it enhances the deterioration of surface RCF layer. In addition, the dislocations induced by the RCF were mostly stemmed from the screw dislocations in the surface RCF layer. In contrast, they were mostly derived from the edge dislocations in the subsurface RCF layer. This difference is likely owing to the characteristics of dislocations, the tangential load, the applied shear stress, localized stress concentration induced by the surface roughness contact, etc.

1. Introduction

In recent years, a lot of research resources have been devoted to the investigation of rolling contact fatigue (RCF) since it is one of the biggest issues faced by railway companies [1–8]. In particular, rail RCF, which is caused by the repeated rolling contact of wheels on the rail, evolves into rail failures such as squats, flaking, head check cracks, etc. These phenomena are costly for mitigation and increase the risk of rail breaks. Railway companies therefore need to employ the inspection and rail grinding to decrease the number of rail failures. These mitigating actions may cause traffic disruptions and capacity reductions. Nonetheless, they may not fully remove the demand for rail replacements due to the rail failures.

So far, intensive numerical simulations of rail RCF have been carried out to quantitatively predict material deterioration and RCF crack propagation to support effective mitigating actions [5–8]. These efforts have significantly progressed the field. However, the complex interacting mechanisms of microstructural refinement, texture formation, anisotropy of deformation, etc. in the RCF layer have made it complicated to fully grasp how the material is deteriorated by the RCF.

Rail steel has some predominant slip crystal planes and direction in its ferrite grain with a body-centered cubic (bcc) crystal structure, which causes anisotropic deformation from a microscopic point of view. In addition, the dislocation movements are complex due to the cross slip. The dislocation density is one of the key material parameters to quantify the degree of plastic deformation. It generally tends to increase as the plastic deformation evolves. This increase of dislocation density induces a grain subdivision such as the formation of dislocation cells, subgrains, high-angle grain boundaries, etc. [9–11], which results in microstructural refinement, plastic flow, texture formation, etc. in the RCF layer. Especially, hardness measurements and texture analyses revealed a drastic microstructural variation in the plastically deformed RCF layer [2,3,12]. Although they are effective in investigating the degree of plastic deformations to some extent, they are not sufficient to provide a thorough understanding of material deterioration in the RCF layer. Most of the RCF related plastic deformation could be attributed to the ferrite grains of the rail steel. This corresponds to the fact that most of the dislocations that accumulate in the ferrite grains owing to the cementite grain in the perlite phase being more brittle than the ferrite grain. Moreover, according to other authors [13], tiny RCF cracks are

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primarily initiated in ferrite grain boundaries. Considering the above, it is desirable to employ a significant measurement method, which quantifies the degree of plastic deformation of the strained ferrite grains in the RCF layer.

In this study, these RCF evaluations were carried out using the x-ray diffraction method. This method has some favorable characteristics regarding the quantification of the RCF affected layer. Firstly, it can be employed to evaluate only the preferentially strained ferrite based on Bragg's law. Secondly, the surface of the RCF layer is measurable. Thirdly, the recent technical and analytical development of the x-ray diffraction method has made it possible to obtain the dislocation density and crystallite size [14–17]. It has been thus applied to many materials such as ultra-fine grained Cu, low-carbon and martensitic steels, etc. and showed good agreement with results from other methods, e.g. transmission electron microscopy (TEM) [17–20]. In the following, we discuss and investigate the applicability of the x-ray diffraction method to the quantification of RCF layers.

2. Experimental analysis

2.1. Serviced rail and RCF test sample preparation for x-ray measurement

Two kinds of serviced Japanese rails were prepared in this study. These rails were in service on tangent tracks in the Japanese network. Accumulated traffic is approximately 500 and 50 MGT (Million Gross Tonnes). In one case, the material deterioration by RCF is expected to be more or less fully developed, whereas in the other case, it is expected to be at an early stage. The rails were manufactured in accordance with the Japanese industrial standard (JIS E 1101) for as-rolled rail. The chemical composition and corresponding mechanical strength for the as-rolled rail are shown in Table 1.

A rail disk sample for a twin disk RCF test was also prepared. It was transversally cut from the head of the as-rolled rail and had the dimension of 50 mm in diameter and 5 mm in thickness. A counterpart disk with the same dimension was also transversally cut from the as-rolled rail head and was thermally treated to give the hardness corresponding to a Japanese wheel. The twin disk RCF test was carried out under the condition of 1.2 GPa in contact pressure, nominal slip ratio of 0%, and dry atmosphere at room temperature. The test consisted of 100,000 cycles.

2.2. Measurement of X-ray diffraction

Small specimens were cut from the tested rail disk and the serviced rails. The x-ray diffraction measurements were carried out below the contact surface in the depth direction. Electrical polishing was employed after each x-ray diffraction measurement to avoid extra stress on the specimen. The number of measuring depths was chosen to include the total thickness of the RCF layer, while at the same time providing sufficiently accurate analyses of the degree of the plastic deformation. CuK_α radiation was employed as an incident x-ray. The x-ray equipment operating at 50 kV and 200 mA picked up only the diffracted CuK_α using the graphite monochrometer mounted at the diffraction side of an x-ray goniometer. The x-ray line profiles corresponding to the crystal planes of (110), (200), (211), (220), (310) and (222) for the ferrite were measured. Each line profile was subjected to a correction process to ensure it consisted only of Cu$K_{\alpha 1}$.

Table 1
Chemical composition and corresponding mechanical strength for the as-rolled rail.

Chemical composition for as-rolled rail as stated in JIS E 1101 (mass%)					Tensile strength (MPa)
C	Si	Mn	P	S	
0.63–0.75	0.15–0.30	0.70–1.10	≤0.030	≤0.025	≥800

2.3. Analysis of X-ray diffraction

The investigation on the estimation of dislocation density using x-ray diffraction was carried thoroughly out [17–20]. Williamson et al. proposed an analysis method to separate the contribution of strain and crystallite size from the x-ray line broadening; the widely known Williamson–Hall equation [21] is

$$\Delta K = \alpha + \varepsilon K \tag{1}$$

with $K=2\sin\theta/\lambda$ and $\Delta K=2\cos\theta(\Delta\theta)/\lambda$ where K, θ and λ are the magnitude of the diffraction vector, the x-ray diffraction angle and the wave length, respectively. ε indicates the strain contribution to the line broadening. α is defined as $1/d$ where d is the crystallite size when the broadening of the x-ray diffraction peak is evaluated by the integral width. The strain, as well as the crystallite sizes will affect the line broadening. Eq. (1) provides us both of these values based on a monotonous function of K. Unfortunately, the strain anisotropy due to the differences in elastic constants is observable in some highly deformed materials and cannot be simply expressed by a monotonous function [17,19,22]. In such cases, the Williamson–Hall analysis would be more suitable as an estimation of strain and crystallite size if strain anisotropy would be suppressed. In fact, with the substitution of ε in Eq. (1) with Hooke's law ($\sigma=\varepsilon E_{hkl}$) it is reported that the material shows more isotropicity stress distribution than in the corresponding strain distribution owing to the modification of K with Young's modulus, E_{hkl}, corresponding to each (hkl) direction and the Miller index of crystal planes [22].

In order to suppress the strain anisotropy observed from the Williamson–Hall analysis, Ungar et al. proposed a modified Williamson–Hall equation through the adoption of new scaling factors consisting of the dislocation contrast factor and the magnitude of the diffraction vector [17]. Assuming that the dislocations mainly contribute to the line broadening caused by strain, the modified Williamson–Hall equation is given by

$$\Delta K = \alpha + \beta K C^{1/2} + O(KC^2) \tag{2}$$

Here C is the dislocation contrast factor determined by the elastic anisotropy constants of a crystal. β and O indicate a constant depending on the effective outer cut-off radius of dislocations and non-interpreted higher-order terms, respectively. C is replaced by the average dislocation contrast factor, $\overline{C}$, which corresponds to each specific (hkl) reflection as follows:

$$\overline{C} = \overline{C}_{h00}(1-qH^2) \tag{3}$$

where $\overline{C}_{h00}$ is the average dislocation contrast factor for (h00) reflections based on the elastic anisotropy constants of a crystal as well as the screw and edge characteristics of dislocations, q is an experimentally determined constant and H^2 is a constant for each specific (hkl) reflection as given by $H^2=(h^2k^2+k^2l^2+l^2h^2)/(h^2+k^2+l^2)^2$. When Eq. (3) is substituted into Eq. (2) and the higher order terms on the right hand side of Eq. (2) are ignored, the modified Williamson–Hall equation is rearranged in the quadratic form as

$$\frac{\Delta K^2-\alpha^2}{K^2} \cong \beta^2\overline{C}_{h00}(1-qH^2) \tag{4}$$

Based on Eq. (4), the q value is experimentally determined by extrapolating $(\Delta K^2-\alpha^2)/K^2$ to high magnitudes of H^2. Note that q is related to the elastic anisotropy constants of a crystal as well as to