Full length article

Understanding cementite dissolution in pearlitic steels subjected to rolling-sliding contact loading: A combined experimental and theoretical study

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ARTICLE INFO

ABSTRACT

Cementite dissolution behavior of pearlitic steels subjected to rolling-sliding contact deformation is comprehensively investigated by combining experimental characterization and phase-field modeling. An elasto-plastic phase-field model, incorporating the elastic strain-induced free energy contribution from first-principles calculations and the plastic counterpart from a rolling-sliding contact finite element model assisted with a plastic strain accumulation model, is originally proposed to simulate the real-time evolution of cementite volume fraction, cementite morphology and carbon distribution for different rolling cycles and contact depths. Upon experimental validations, the proposed model predicts more accurate and realistic results than Sauvage's model. A three-stage behavior of cementite dissolution is also revealed, which well explains an experimentally observed significant cementite dissolution gradient along the depth direction. Besides, the effect of ferrite/cementite interface thickness and the initial lamellae thickness of cementite on cementite dissolution kinetics is studied. The proposed phase-field model can not only help understand the mechanism of cementite dissolution, but also give new sights into quantitative predictions of the mechanical properties and even the rolling contact fatigue life of pearlitic rail steels in service.

Published by Elsevier Ltd on behalf of Acta Materialia Inc.

1. Introduction

Rails are subjected to increasing mechanical wear and rolling contact fatigue (RCF) due to fast train speed [1] and massive axle loads [2] in modern railway systems. Therefore, there are surging interests to explore the underlying mechanism of material failures for improving the properties of existing rail steels and prolonging the service life of rails. Microstructure evolution in the surface layer of pearlitic rail steels has been well recognized to be closely related to the degradation of mechanical properties, the formation of microcracks, and eventually failure in rails [3,4]. For example, White Etching Layer (WEL), a hard and brittle layer featured with so called "cementite dissolution" in the microstructure on rail surface is usually believed to be favorable locations of crack initiation, which is dramatically detrimental to the rail lifetime [5,6]. However, the details of microstructure evolution in pearlitic rail steels during rolling-sliding contact deformation, including pearlite deformation, grain refinement of ferrite and especially dissolution of cementite, remains elusive due to the complicated interaction between the cyclic contact load, the frictional heat and complex microstructure characteristics. Therefore, there is currently a critical need to understand the fundamental mechanism of microstructure evolution of rail steels under rolling-sliding contact deformation.

A great number of experimental efforts have been made on microstructure characterization of rail surface during the past

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decades. Most of the experimental observations are focused on finding the evidences to support two categories of cementite dissolution mechanisms that are still in dispute, i.e., mechanical deformation induced dissolution vs. heat induced dissolution. Wild et al. [7] claimed that cementite dissolution was caused by frictional heat induced austenization and subsequent martensitic transformation, based on the experimentally observed retained austenite in rail surface. Takahashi et al. [8] estimated the temperature rise in rail surface from the concentration profile of Mn measured by three-dimensional atom probe (3DAP). They concluded that the temperature could reach 1300 °C at the topmost surface, which suggested that cementite dissolution occurred during rapid austenization caused by frictional heat. However, Fischer et al. [9] found that flash temperature could not exceed 500 °C even at the condition of maximum contact stress of 1500 MPa, 5% sliding ratio and velocity of 50 m/s. Considering that the austenitization temperature for eutectoid steel is 740 °C and does not decrease to less than 500 °C even at a much higher hydrostatic pressure [10], the austenitization by the temperature rise during normal rail–wheel contact conditions is not convincing [6]. Therefore, we tend to think that the austenite observed may be formed under some accidental extreme conditions, such as sudden brake [8], which can cause an enough local temperature rise for austenization. With increasing evidences in severe plastic deformation induced cementite dissolution by high pressure torsion [11] and cold drawing [12], Lojkowski et al. [13] proposed that the mechanism of cementite dissolution in rail surface was more likely driven by the severe plastic deformation. More specifically, they stated that the transformation can take place at a temperature of less than 230 °C after cyclic rolling-sliding contact deformation. By eliminating the effect of frictional heat, Chen et al. [14] recently confirmed that the cementite dissolution is caused by cyclic plastic deformation rather than frictional heat induced austenization under their experimental parameters. Although the mechanism of cementite dissolution under rolling-sliding condition is still a highly controversial issue, it is reasonable to postulate that mechanical deformation is one of the dominant factors under most experimental conditions.

Tremendous research works have been performed to understand how mechanical deformation drives cementite dissolution. As reviewed in Ref. [15], there are generally two potential underpinnings of cementite dissolution under severe loadings. Gridnev et al. [16,17] proposed that the cementite dissolution may be induced by the difference between the binding energy of carbon interstitials and dislocations and the binding energy of carbon atoms and iron atoms in cementite under mechanical deformation. On the other hand, Languillaume et al. [18] thought that cementite dissolution is possibly contributed by the increase of free energy of cementite from thinning of cementite lamellae and formation of slip steps caused by plastic deformation. By extending Languillaume's model, Sauvage et al. [19] semi-quantitatively calculated cementite dissolution rate in cold-drawn pearlitic wires based on a diffusion-controlled dissolution process. Unfortunately, the predicted dissolution rates appeared to be underestimated in comparison with the experimental measurements. Further, the work was limited to cold-drawn pearlitic wires and cold-worked pearlitic steels in which the mechanical deformation is applied in

the fashion of only one or a few cycles. Pearlitic rail steels, however, have to endure thousands of rolling-sliding contact deformation cycles during service. The cementite dissolution behaviors in pearlitic rail steels under cyclic loading may differ significantly from that in the simply cold-drawn pearlitic wires.

More recently, Nematollahi et al. [20] suggested that in addition to the contribution from the plastic deformation, an elastic strain-tuned free energy can be another potential contributor to cementite dissolution according to first-principles calculations. However, all of these existing studies are still at the early "hypothetical" stage where at most, only semi-quantitative calculations were conducted on the cementite dissolution of pearlitic steels. A reliable model integrating such two factors and how these two factors intrinsically contribute to the cementite dissolution is still not available.

In the present study, an elasto-plastic phase-field model, integrating an elastic strain and plastic strain induced free energy increase in cementite and ferrite, is originally proposed to understand the fundamental mechanism of mechanical deformation induced cementite dissolution. Upon the experimental validation, the proposed model has been demonstrated to achieve a quantitative estimation of cementite dissolution kinetics in cold-drawn pearlitic wires. The validated model is then applied to a pearlitic steel under cyclic rolling-sliding contact deformation. The simulated cementite volume fraction, cementite morphology and carbon distribution are then directly compared with the results after rolling-sliding contact experiments. The present elasto-plastic phase-field model is applicable to the cementite dissolution in pearlitic steels under various manufacturing or serving conditions.

2. Experimental methods

A hypereutectoid pearlitic steel is used in the present study; the details of heat treatment and experimental setup are given in Ref. [14]. Torque and friction coefficients are recorded by torque transducer and are then used as input parameters for the rolling-sliding contact finite element model. Table 1 lists the rolling-sliding contact experimental parameters in the present study. The applied load is 1500 N, and the sliding ratio between the up and bottom discs is 0.5%. The only different parameter between sample A and sample B is the number of rolling cycles, which is 30000 cycles for sample A and 120000 cycles for sample B.

After rolling-sliding contact experiments, longitudinal sections of the discs are prepared for scanning electron microscopy (SEM) through mechanical grinding and polishing followed by etching in 4% solution of HNO_3 in ethanol. Transmission electron microscopy (TEM) samples at different depths below the contact surface are prepared by focused ion beam (FIB). TEM characterization is conducted on JEM-2100 F with an operating voltage of 200 kV.

3. Model description

In this study, a multiscale computational framework, in which an elasto-plastic phase-field model is coupled with the finite-element method, is proposed to model the cyclic mechanical deformation-driven cementite dissolution. The distributions of stress and strain as functions of rolling cycles and contact depths, at

Table 1
Experiment parameters of rolling-sliding contact conditions.

Sample	Load (N)	Up disc speed (rpm)	Bottom disc speed (rpm)	Sliding Ratio (%)	Rolling cycles
A	1500	500	497.5	0.5	30000
B	1500	500	497.5	0.5	120000