Modeling of hydrogen transport in rolling contact fatigue conditions

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Abstract

Current work presents Finite Elements study of hydrogen diffusion into a metal substrate loaded by rolling contact. The main goal of the presented study is to investigate stress effect on hydrogen transport in rolling contact conditions. In this work, rolling contact is defined by the Hertzian pressure, moving along the bearing ring. Although, hydrogen diffusion with respect to bearing is studied here, very similar approach can be used for other components of machinery subjected to rolling contact. Governing equations are given in the current study in dimensionless form, and parametric study, analyzing influence of different dimensionless parameters on subsurface concentration of hydrogen, is presented.

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1. Introduction

Rolling contact fatigue (RCF) is driven by different mechanisms of material degradation: mechanical damage (crack initiation and propagation), phase transformation, corrosion and hydrogen diffusion. The latest is known to be very detrimental to the mechanical properties of steel. Hydrogen atoms being extremely small can easily penetrate into steel - the phenomenon, known as the hydrogen ingress. Hydrogen leads to reduction of material toughness (embrittlement), which enhances crack propagation in RCF.

In rolling contact fatigue conditions, the source of hydrogen is expected to be mainly from the reaction of water at the metal surface or from the decomposition of the lubricant [1]. The mechanism is described to be a catalytic reaction of hydrocarbon lubricants with the fresh surface of the steel [2].

The typical RCF failure related to hydrogen is so-called brittle flaking which is frequently accompanied by white etching areas. The role of hydrogen has become evident from observations of flaking damage in bearing components where the measured amount of hydrogen was high and from observation of the same type of failure in test rig specimens, which were pre-charged by hydrogen. A subsurface crack surrounded by white etching area [3] is shown in Fig. 1.
In [4] the amount of hydrogen measured in inner rings, outer rings and balls of bearing run under acceleration-deceleration tests, was highest in the stationary ring, where brittle flaking was likely to occur. In [5] the hydrogen charged specimens were run in the trust bearing RCF test rig, showing that the flaking life decreases with the growing amount of pre-charged hydrogen. The tension-compression and RCF properties of bearing steel were investigated in [6] under various hydrogen pre-charging conditions. The results of [6] demonstrated that the decrease of the fatigue strength was in direct correlation with the diffusible hydrogen content. The RCF test conducted in [6] showed that the crack initiation life decreased as the amount of the diffusible hydrogen increased.

The hydrogen enhanced brittle failure (like flaking in RCF) can be associated with the reduction of the surface energy (cohesive strength) by hydrogen absorption – the fact proven experimentally [7] and theoretically [8], by the first principle computations. The surface energy, as known, is strongly related to resistance of material to crack propagation; therefore reduction of surface energy leads to steel embrittlement by decreasing of the toughness and the fatigue crack threshold, $K_{th}$. The dramatic reduction of the latter property due to growing amount of diffused hydrogen was demonstrated experimentally for ultrahigh strength steel [9]. The hydrogen embrittlement can be also presented in terms of fatigue limit reduction, as was proposed in [10], where the fatigue strength of steel was multiplied by the hydrogen influence factor. Note, that if the hydrogen embrittlement effect is involved in fatigue process, then a theoretical model for RCF should evaluate the distribution of hydrogen below the rolling surface (for estimation of $K_{th}$ or fatigue limit reduction), along with the crack analysis.

Concentration of diffused hydrogen in steel can be evaluated in terms of continuum approach by solving of mass diffusion equation (Fick’s law), which in the case of stressed components has to include the stress-diffusion term defining the transport of hydrogen induced by the gradient of hydrostatic stress. In literature, many theoretical studies for hydrogen diffusion into stressed components, based on continuum approach can be found. As example, hydrogen diffusion into the pressure vessel wall was studied in [11] and in notched bar specimen in [12] and [13] by Finite Elements (FE). However, no any theoretical study, describing hydrogen diffusion in rolling contact conditions was found. In the current work the numerical code, based on FE, for solution of diffusion equation was developed and parametric study demonstrating hydrogen concentration profiles vs. different dimensionless parameters was presented. The main focus of this work is the investigation of stress effect on the hydrogen transport in rolling contact conditions. Based on the proposed study, the amount of subsurface hydrogen as the function of time and other parameters, like material properties and rolling contact conditions, can be estimated. And later relating the hydrogen concentration to the steel brittleness RCF life based on stress analysis or fracture mechanics can be predicted.
2. Background

The governing equation of transient hydrogen diffusion in metals which accounts for the hydrostatic stress, $p$, effect, is (see e.g. [13]):

$$\frac{\partial C}{\partial t} = D \nabla^2 C + \kappa \nabla \cdot \left( C \nabla p \right) \quad \text{where} \quad \kappa = \frac{D V_H}{RT}$$  \hspace{1cm} (1)

Where $C$ is the hydrogen concentration, $D$ - the hydrogen diffusion constant, $V_H$ - the partial molar volume of hydrogen in solid solution, $R$ - the gas constant and $T$ - the absolute temperature (in Kelvin). Recall, that the hydrostatic stress, $p$, is defined as $3 \left( \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3} \right)$, where $\sigma_{xx}$, $\sigma_{yy}$ and $\sigma_{zz}$ are the normal stresses in $x$, $y$, and $z$ directions, respectively. The first term in the right-hand-side of Eq. (1) defines the hydrogen diffusivity due to the gradient of concentration (governed by the diffusion constant, $D$) and the second – due to the gradient of hydrostatic stress (governed by the stress-diffusion constant, $\kappa$).

It is important to note that Eq. (1) provides the simplest way to describe mathematically the complicated process of hydrogen transport into metals. This simple equation does not describe explicitly the trapping of hydrogen atoms by material imperfections (vacancies, dislocations). To account this effect properly, more advanced diffusion models, like McNabb-Foster [14] or Sofronis [15] equation, should be used, instead. The former model includes additional equations describing migration of hydrogen from lattice to traps (and backward), and the latter model assumes that the diffusion constant is dependent on the hydrogen concentration. For the current modeling (based on Eq. (2)), the diffusion constant can be experimentally measured in permeation test [16], where the, so-called, effective $D$, incorporating diffusible and trapped hydrogen can be identified.

3. Diffusion in rolling contact

In rolling contact, hydrogen diffusion process is influenced by subsurface cyclic stresses produced by moving contact pressures, which are formed at the contact between rolling elements (e.g. rollers, balls) and substrate (e.g. inner ring of bearing). Schematically, it is shown in Fig. 2, where the material domain loaded by moving contact pressures and parameters defining geometry and boundary conditions are presented. The stress-diffusion problem is considered as two-dimensional, which means that stress calculations are based on the plane-strain conditions.

As is presented in Fig. 2, the contact load is described by the Hertzian distribution which is defined by the two parameters [17]: the contact zone semi-width, $b$, and the maximum contact pressure, $p_0$. The distance between the two contact zones (or between the two rolling elements) is denoted by $l$; the linear velocity of the contact zones propagation along the raceway is $V$. The boundary conditions governing the diffusion process are given in terms of the hydrogen concentration on the two surfaces of the ring. The high concentration, $C_{s}$, is defined on the raceway (rolling surface), where hydrogen is generated by lubricant and water decomposition, and the vanishingly low concentration, $C_{h}$, on the opposite surface of the ring. Typically, this surface is in a contact with another machinery component (e.g. shaft in the case of inner ring of bearing). The distance between the two surfaces, $h$, is the thickness of the ring.
Special attention regarding boundary conditions should be paid in the current problem. As is schematically presented in Fig. 2, the hydrogen concentration on the raceway (boundary condition) is not uniform, but is dependent on the position of the contact load. This is because the surface hydrogen concentrations below and out of the contact zone are not identical. When lubricant is below the contact it is subjected to high temperature, pressure and friction, which can cause decomposition of lubricant and hydrogen generation. It means that the hydrogen concentration below the contact should be somewhat higher than out of it; however experimental measurement of this difference is extremely difficult if not impossible. Hence, in the current work, this effect is introduced artificially, by the parameter, $c_H$ (subscript “$H$” relates to the word Hertzian), defining the peak value of concentration (see Fig. 2). At the center of the contact (below $p_0$) it reaches maximum, and is $c_H$ time higher than the background hydrogen concentration, $C_0$. Similarly to the contact pressure, the hydrogen concentration distribution propagates along the raceway together with the rolling element (at the velocity $V$). If $c_H$ is chosen to be 0, then the hydrogen concentration on the surface is uniform and equals to $C_0$. Finally note that $c_H$ dependent on $p_0$, friction coefficient ($\mu$) and possibly on other parameters defining the lubrication and contact conditions (e.g. roughness, film thickness, slip-to-roll ratio, etc).

Figure 2. Schematic of the hydrogen diffusion problem under rolling contact conditions
Now, let developed Eq. (1) for the two-dimensional diffusion problem, schematically presented in Fig. 2:

$$\frac{\partial C}{\partial t} = D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2} \right) + \kappa \left( \frac{\partial C}{\partial x} \frac{\partial p}{\partial x} + \frac{\partial C}{\partial z} \frac{\partial p}{\partial z} \right) + \kappa C \left( \frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial z^2} \right)$$

(2)

It is important to note, that in the rolling contact problem, the hydrostatic stress, $p$, and its derivatives are not only functions of $x$ and $z$ coordinates, but are time dependent, too. This is because the contact pressures, loading the bearing ring are not static, but propagate along the surface of the solution domain (as is schematically shown in Fig. 2), which leads to the stress alternation in time. In the case of plane strain, the hydrostatic stress is defined by the function of the two coordinates: the subsurface depth, $z$, and the equivalent coordinate $x + Vt$, which accounts for the propagation of contact pressures. The hydrostatic stress function is periodic with respect to $x + Vt$ and the period of this function (assuming that the time, $t$, is fixed) equals to $l$ which is the distance between the two rolling elements. On the other hand, if one assumes that the coordinate $x$ is fixed (e.g. $x=0$), he will get that the hydrostatic stress function is periodic with respect to time, and the time-period is $l/V$.

The fact, that the hydrostatic stress distribution in the rolling contact diffusion problem is time dependent, leads to serious difficulty to solve this problem numerically. This is because the two time-scales govern this stress-diffusion problem, and these time-scales are very different from each other. The first time-scale corresponds to the “diffusion time” or the natural time governing the hydrogen diffusion into solid without any stress effect. This natural time can be defined as $h^2/D$, and it indicates how fast the ring will be saturated by hydrogen (steady-state solution). The second time-scale corresponds to the “stress cycle time”, and this time can be defined as the period of the stress alternation, caused by the motion of rolling elements. This time-scale is included into the stress-diffusion problem by the two last terms of Eq. (2), and can be defined as $l/V$, or as the time required for one over-roll. It is obvious, that the two aforementioned time-scales are very different from each other. The “diffusion time” corresponds to slow diffusion process, while the “stress cycle time” to very rapid stress alternation in operating bearing, or in the other words: $h^2/D >> l/V$. This difference between the two time-scales can lead to the tremendous number of solution steps, in attempt to solve this problem numerically and to long computational time.

4. Simplification of rolling contact problem

The numerical simulation of diffusion problem in rolling contact conditions is time consuming, however, solution time can be shortened by reducing dimensionality of the problem domain (from 2D to 1D). Considering stress alternation at subsurface points of ring, located at the same depth, one can easily indicate, that all these points are subjected to the same stress history. Obviously, it is true only in the case of a bearing which rings are loaded by moving contact pressures, of the same $b$ and $p_{th}$, and where the effect of the non-equal load distribution along the ring (due to external load or gravity) is neglected. In this case, the points located at the same subsurface depth will undergo the same stress-diffusion process, and the concentration of subsurface hydrogen will be mainly dependent on time and the depth coordinate, while the dependence on the $x$-coordinate will be almost negligible. Alternating hydrostatic stress can cause only to cyclic hydrogen diffusion along the $x$-coordinate (from left-to-right and from right-to-left), however in average, its transport in this direction is zero. It means that the two-dimensional rolling contact diffusion problem can be reasonably simplified to one-dimensional, neglecting the hydrogen transport along the $x$-coordinate. It is also important to note, that by this simplification other stresses, like hoop and residual stress [18], being dependent solely on subsurface depth and independent on circumferential coordinate and time, can be accounted for the stress-diffusion analysis, along with time-dependent Hertzian stresses.

Neglecting hydrogen transport in $x$-direction leads to considerable simplification of Eq. (2):

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2} + \kappa \left( \frac{\partial C}{\partial z} \right) f_1(z, t) + \kappa C f_2(z, t)$$

(3)

which is now dependent on the time and single coordinate, $z$. The two functions in Eq. (3) $f_1(z, t)$ and $f_2(z, t)$ are derived from the hydrostatic stress, $p$. As follows from Eq. (2): $f_1 = \frac{\partial p}{\partial z}$ and $f_2 = \frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial z^2}$. Eq. (3) can be presented in dimensionless form, and for this the following set of normalized parameters should be
defined: the dimensionless time \(- \tilde{t} = t/(l/V)\), the dimensionless hydrogen concentration \(- \tilde{C} = C/C_0 \), the dimensionless hydrostatic stress \(- \tilde{p} = p/p_0 \), the dimensionless distance between the two rolling elements \(- \tilde{b} = l/b \), the dimensionless ring thickness \(- \tilde{h} = h/b \), the dimensionless z-coordinate \(- \tilde{z} = z/b \), the dimensionless x-coordinate: \(\tilde{x} = x/b\), the dimensionless \(f_1\)-function \(- \tilde{f}_1 = f_1/(p_0/b)\) and the dimensionless \(f_2\)-function \(- \tilde{f}_2 = f_2/(p_0/b^2)\). Substituting these dimensionless parameters into Eq. (3) the following dimensionless equation is obtained:

\[
\frac{\partial \tilde{C}}{\partial \tilde{t}} = \xi \frac{\partial^2 \tilde{C}}{\partial \tilde{z}^2} + \psi \left( \frac{\partial \tilde{C}}{\partial \tilde{z}} \right) \tilde{f}_1 + \psi \tilde{C} \tilde{f}_2
\]  

(4)

Eq. (4) is governed by the two dimensionless parameters \(\xi\) and \(\psi\) which can be termed the dimensionless diffusion and stress-diffusion constants in rolling contact, respectively.

These two parameters are defined in the following way: \(\xi = \frac{Dl}{Vb^2}\) and \(\psi = \frac{Dl}{Vb^2} \frac{p_0 V_H}{RT} = \xi \frac{p_0 V_H}{RT}\).

The boundary and the initial conditions for Eq. (4) are also presented in dimensionless form:

\[\tilde{C}(\tilde{z} = 0) = \tilde{C}_0(\tilde{t}) \text{ and } \tilde{C}(\tilde{z} = \tilde{h}) = 0\]  

(5)

\[\tilde{C}(\tilde{t} = 0) = \tilde{g}(\tilde{z})\]  

(6)

Eq. (5) defines the dimensionless boundary conditions for one-dimensional solution domain; on the surface the hydrogen concentration is given by the time dependent periodic function \(\tilde{C}_0\) (if the \(c_H\) parameter vanishes then \(\tilde{C}_0 = 1\)) and at the depth \(\tilde{h}\) for simplicity assumed to be 0. The initial conditions are given by Eq. (6) in terms of the dimensionless function \(\tilde{g}(\tilde{z})\) which defines the initial concentration of hydrogen (normalized by \(C_0\)) in the solution domain.

Eqs. (4-6), describing dimensionless stress-diffusion problem, are solved here numerically, by the FE program, developed in MATLAB. Subsurface stresses are evaluated semi-analytically by the integration of the Flamant solution (concentrated force acting on an elastic half-plane [17]) over the Hertzian contact pressure distribution.

5. Results

Using FE code, the aforementioned stress-diffusion problem in dimensionless form is solved, and the results of the parametric study are presented in the current section.

In Fig. 3, the effect of dimensionless diffusion constant, \(\xi\), on the hydrogen transport is presented. To investigate the effect of \(\xi\) on diffusion separately from other parameters, the values of \(\psi\) and \(c_H\) are assumed to be 0, which means that the uniform hydrogen concentration \(C_0\) is defined on the surface (boundary condition), and that the domain is free of stress. It should be noted, that the dimensionless diffusion constant being defined as \(Dl/Vb^2\) can practically get any value, depending on the velocity \(V\) and \(l/b\) ratio (high dimensionless values of \(\xi\) correspond to slowly running bearing).
The hydrogen concentration profiles in Fig. 3, are presented, for a wide range of $\xi$, varying from $10^{-5}$ to $10^{-2}$. As is shown in this figure, $\xi$ has strong effect on the diffusion process: in the case of high $\xi$ values hydrogen transport is much faster than in the case of low $\xi$ values. Such dependence is expectable, because high values of the dimensionless parameter $\xi$, correspond firstly do high values of $D$ (defining the diffusion speed in absolute units) and secondly to low values of $V$. It is important to note that the latter parameter has no direct effect on the diffusion process (when solution domain is stress free), however this parameter defines the dimensionless time $\tilde{t}$. It means that for two bearings running at low and high speeds, the same $\tilde{t}$ value can corresponds to very different absolute times: for the slow bearing the absolute time (and therefore $\xi$ value) is higher than for the fast one.

The stress effect on hydrogen transport in rolling contact is governed by the dimensionless stress-diffusion constant $\psi$, and the parametric study of this effect is presented in Fig. 4. In order to get pronounced influence of stress on diffusion, the amount of subsurface hydrogen has to be sufficiently high, because hydrogen flux due to hydrostatic stress gradient, as follows from Eq. (1), is proportional to concentration. It means that after short time, when the concentration of hydrogen is rather low, the stress effect on diffusion is vanishingly small, so in order to get considerable influence of stress on diffusion process the amount of subsurface hydrogen has to be sufficiently high.

On the other hand, as was mentioned in the Section 3, numerical simulation of diffusion process is very computational expensive in rolling contact due to large number of solution steps. Hence to be able to detect the stress effect on hydrogen transport without spending enormously long computational time, a very thin ring (which thickness, $h$, is only three times larger than $b$) is taken for simulation.
As is shown in Fig. 4, the amount of subsurface hydrogen increases as stress-diffusion constant \( \psi \) goes up, and it means that subsurface stress in rolling contact enhances diffusion of hydrogen, by “infusing” it from surface to subsurface. Recall, that \( \psi / \xi = p_0 \nu_H / RT \) and special note regarding numerical values of this ratio should be done. Practically, this ratio varies in rather narrow range of values. The partial molar volume of hydrogen, \( \nu_H \), is about 2000 mm\(^3\)/mol for steels (and is close to this value for other metals) [19] and the gas constant \( R \) as is well known, is 8.31432 J/(mol.K). The typical values of \( p_0 \) are in the range of 2 to 3.5 GPa (the latter high value is typical for hybrid bearings, in which rolling elements are made of ceramics). It means, that at the room temperature (\( T = 20 \) °C or \( \approx 293 \) K) \( \psi / \xi \) is in the range of 1.5 to 3. To get significantly higher \( \psi / \xi \) values, the maximum contact pressure, \( p_0 \), has to be unrealistically high or/and the temperature, \( T \), extremely low. It means that the results presented in Fig. 4 for \( \psi = 3 \) and 1.5 (when \( \xi = 0.01 \)) correspond to enormously high values of the \( \psi / \xi \) ratio. On the other hand, numerical simulation showed that in the range of 1.5 \( < \psi / \xi < 3 \), the effect of stress on hydrogen transport is negligible (concentration profiles for such conditions simply coincide with the profile of the reference case, \( \psi = 0 \)).

Why the stress effect on hydrogen transport in rolling contact is so subtle, can be explained by Fig. 5. This figure presents dimensionless distributions of subsurface hydrostatic stress (which enhances diffusion) below the two neighboring contact zones. The hydrostatic stress distributions as the functions of \( x/b \) are shown in Fig. 5 for the three different dimensionless depths: \( z/b = 0.05, 0.5 \) and 2. The hydrostatic stress, as is indicated by this figure, is peaked at low depth, and as the depth increases the distribution of hydrostatic stress decays and smears. However, the most important observation which one can get from Fig. 5 is that the subsurface material below the two contact zones is predominantly unloaded: subsurface stress is concentrated at the contact zones, while the rest of the material is free of stress (note that \( x/b \) in the range of 10 to 90 where \( p \) is practically 0, is omitted from Fig. 5). It means, that the average hydrostatic stress in the ring, \( \frac{1}{L} \int_{l/2}^{l/2} p(x) dx \), is rather low and as result the effect of stress on hydrogen transport is negligible. It occurs, because the size of the contact zone, that \( b \), is much smaller than the distance \( l \), which at least equals to the diameter of a rolling element \( d \) (see again Fig. 5). In the other words, the time in which hydrogen diffusion is enhanced by stress, is relatively very short compared to the total diffusion time (most of the time the ring is unloaded).
Finally, the effect of non-uniform boundary conditions along a raceway in rolling contact is studied. As was mentioned in the Section 3, generation of reactive hydrogen on a surface of ring in bearing is dependent on multiple contact conditions, and therefore it is reasonable to presume, that the hydrogen concentration at the contact zone is somewhat higher than out of it. This effect is included by parameter $c_H$, and the concentration profiles for different values of this parameter are shown in Fig. 6. As is shown in this figure, increasing of $c_H$ values from 0 to 25 (see again explanation in Fig. 2), produce higher concentration of hydrogen below the surface. Similarly to the stress induced diffusion, the effect of increased concentration of hydrogen below the contact, is active only when the solution domain is passed by contact.

6. Conclusions

Hydrogen transport into a ring of bearing stressed by moving contact loads was investigated numerically in the presented study. For this FE model for simulation of hydrogen diffusion under rolling contact conditions was developed. The main numerical difficulty related to the two different time-scales in the rolling contact problem was discussed and methodology simplifying this problem by reduction of its dimensionality was proposed. The equations describing diffusion of hydrogen in stressed material were normalized and a parametric study analyzing the influence of different dimensionless parameters on the subsurface concentration of hydrogen in rolling contact conditions was presented. The parametric study indicated that subsurface stress produced by moving rolling elements has vanishingly small effect on diffusion of hydrogen, and this occurs because high stresses are concentrated only at the contact zones, while the major part of the ring volume remains free of stress. Such conclusion leads to considerable simplification of problem, meaning that time dependent subsurface stress produced by rolling elements can be neglected and the second time-scale can be safely excluded from analysis. However it does not mean that the stress effect on hydrogen transport can be totally removed from the study: as was mentioned in the Section 4, bearing rings can be subjected to other stress, like residual or hoop stress, which are constant with respect to time, and have therefore non-negligible effect on diffusion process. Hence, in the next study these stresses should be accounted for. Also, future study should focus more on material modeling by using advanced diffusion equations, describing properly behavior of lattice and trapped hydrogen.
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