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Hydrogen diffusion and trapping in bodies undergoing rolling contact

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ABSTRACT

Diffusion and trapping of hydrogen (H) in bodies undergoing combined rolling and sliding contact has been evaluated using finite element analysis. The elastic stress–strain conditions of the bodies were calculated in 3D for a single rotation. The stresses were then used to simulate H diffusion in a single plane close to the contact point over large numbers of cycles. The distribution of deformation-induced defects was approximated by relating an isotropic hardening model to the dislocation density. The influence of the defects on H diffusion was evaluated using the McNabb & Foster model assuming local equilibrium as per Oriani. The influence of residual stresses, such as those occurring in bearings after manufacturing, and frictional heating were also considered. The results show that slightly elevated H concentrations occur in the plastic zone conditions and that the increase in H concentration is due to trapping by deformation-induced defects. The influence of stress-assisted diffusion is small due to (i) the short period of time a point on the contact surface spends under load relative to the period of rotation; and (ii) the spatial separation of the hydrostatic and von Mises components of the contact stresses.

1. Introduction

Hydrogen-assisted rolling contact fatigue (HA-RCF) is often proposed as a cause of premature degradation of rolling element bearings by "brittle flaking" or "white structure flaking". There is a consensus in the literature that hydrogen is generated by degradation of the lubricant by some tribo-chemical reaction [1–6] and absorbed by the bearing material as atomic hydrogen (H). However, there is general disagreement regarding the mechanism that promotes the H generation and ad/absorption (a prevailing proposal is that the critical process is the catalysis of the decomposition reaction by bare metal surfaces exposed by sliding contact [2]) and the influence of H on fatigue damage processes. Critical to understanding the latter is developing an understanding of the diffusion and trapping of H inside the bearing material. Due to the complicated natures of the contact stresses and the distribution of deformation-induced defects that may act as H traps, this is less intuitive than other problems involving stress-assisted H diffusion. For example, continuum models have shown that H accumulates at regions of elevated tensile stresses such as those occurring around crack tips [7–11]. In contrast, contact stresses are mostly compressive in nature and thus tend to repel H. This is further complicated by the existence of residual stresses resulting from machining and hardening processes, which may be compressive or tensile. Disregarding the influence of H traps, it is not immediately clear why H should remain, let alone accumulate, in the region where fatigue damage processes are occurring. Thus, it was anticipated that deformation-induced defects acting as H traps would have a considerable influence on the H-distribution in bodies undergoing rolling contact.

The aim of the described work was to provide a preliminary analysis of stress-assisted H diffusion and trapping under conditions typical of those occurring in bodies undergoing rolling contact. We chose to simulate experiments currently being carried out at IWM using double-roller type specimens, in which premature rolling contact fatigue failure has been shown to occur for H-charged samples and for which test parameters were available. One of the challenges associated with simulation of such systems is the competing demands of modelling of the stress–strain condition and of H diffusion and trapping. Although analytical solutions for the elastic stress condition of the material exist [12–16], these are complex and do not consider the combined influences of rolling and sliding contact. A more accurate depiction of the stress–strain state requires a detailed 3-dimensional discretisation of the specimen geometry, the solutions to which are computationally intensive. In contrast, modelling of H diffusion and trapping over large numbers of cycles requires very high computational expediency. In the present work, this conflict was resolved through the implementation of a multiscale framework, in which the elastic stresses were calculated in 3D using ABAQUS for a single rotation and exported along with the nodal data into

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a bespoke FE code programmed in Python for determining the distribution of H in a single radial plane under isothermal conditions over large numbers of cycles. This spatial separation of the stress and H diffusion problems necessitated the assumption that the hardening behaviour of the material follows an isotropic hardening power-law. A consequence of this assumption is that a steady-state distribution of defects is attained after the first few rotations (the “shakedown” period), and remains constant throughout the period of H diffusion. The results, though not constituting a thorough treatment of plasticity effects, show that the H-distribution in the near-contact region is relatively constant, with slight increases in H concentration due to H trapping at deformation-induced defects.

2. Details of model

2.1. Evaluation of the stress–strain condition

Rolling contact stresses were calculated for a twin-disc test configuration using a coupled thermal-mechanical three-dimensional finite element simulation in ABAQUS. Due to the symmetry of the system, only one-half of the geometry was modelled. The model was comprised of a crowned disc with a circular profile rolling on the surface of a flat roller with a predefined normal force and slip rate under continuous oil lubrication. The dimensions of the rollers are shown in Fig. 1. The disc and roller were rotated at 300 and 270 rpm respectively, i.e. with a slip ratio of approximately $s=0.105$, under a constant normal load of 1 kN.

Coulomb friction with a constant frictional coefficient of $\mu=0.08$ was assumed based on the average frictional coefficient determined through a series of measurements carried out using a twin-disc tribometer. Isotropic linear elastic material behaviour for 100Cr6 (SAE52100) steel was assumed for both bodies. This ensured an adequate approximation of a quasi-Hertzian contact condition.

In order to resolve contact stresses with an acceptable accuracy while maintaining a reasonable size, a dense mesh was created in the vicinity of the contact surfaces only. The average element size adjacent to the plane of symmetry was $60 \times 60 \times 20$ μm. Eight-node first-order hexahedral elements with displacement and temperature degrees of freedom (C3D8T) were used to discretise the geometry.

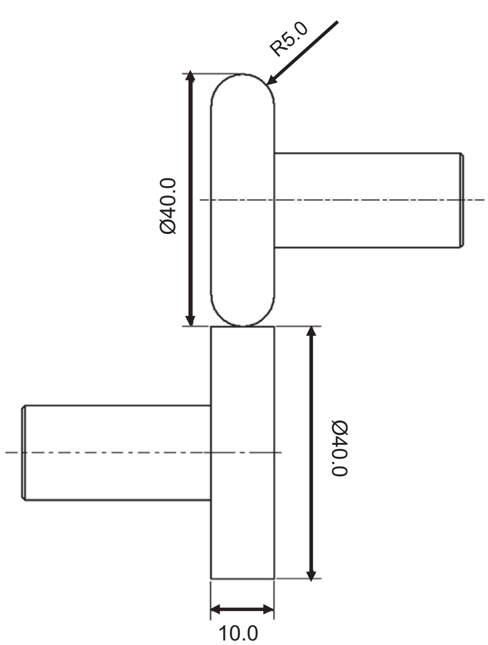

Fig. 1. Dimensions of the crowned and flat roller (millimeter).

The frictional energy dissipation was calculated from the frictional stress and slip rate. The distribution of the heat between the interacting surfaces was assumed to be identical, whereas the fraction of dissipated energy converted into heat (mechanical to thermal) was assumed to be 90% of the overall frictional energy, in order to account for heat transfer losses by natural convection and lubrication. Thermo-mechanical properties were linearly interpreted from those listed in Table 1.

The nodal data (coordinates and stresses) were extracted from a plane parallel to a cutting surface along the cross section of the contact ellipse (X–Y plane in Fig. 2) and exported into the H diffusion model.

2.2. Hydrogen diffusion and trapping model

Detailed descriptions of the finite element formulation of H diffusion and trapping are given elsewhere [7–11]. Here only a brief overview will be given in order to outline the key differences between the past and present routines.

2.2.1. Hydrogen diffusion

The simplest formulation of H diffusion in a stressed lattice in the presence of traps is derived by assuming local equilibrium between H in trap sites and in the surrounding lattice. This assumption enables the H concentration of traps, C_T, to be written as a function of the local lattice concentration, C_L. Thus, in order to describe the macroscopic redistribution of H in the entire system we need only to describe the rate of change of C_L. Assuming isothermal conditions, this is given by [17–19]:

$$\frac{dC_L}{dt} = D_{eff}\left(\nabla^2 C_L - \nabla C_L \nabla^2 \sigma_{kk} \frac{V_H}{3kT}\right) \tag{1}$$

where σ_{kk} is the hydrostatic component of the stress, V_H is the partial molar volume of H in solid solution with the bulk lattice and D_{eff} is an effective diffusion coefficient, which is given by:

$$D_{eff} = D_L \frac{C_L}{C_L + C_T(1-\theta_T)} \tag{2}$$

where D_L is the diffusivity of H in the trap-free lattice and θ_T is the ratio of trapped H atoms to trap sites (i.e. C_T/N_T), which is in turn given by:

$$\theta_T = \frac{1}{(1 + (1/K_T\theta_L))} \tag{3}$$

In which θ_L is the occupancy of lattice sites by H (i.e. C_L/N_L) and K_T is the so-called equilibrium constant. K_T may be defined as the ratio of the characteristic frequencies of H atoms jumping from traps to lattice sites, λ, and from lattice to trap sites, κ, and is given by the Arrhenius expression:

$$K_T = \frac{\kappa}{\lambda} = e^{-\Delta E_T/RT} \tag{4}$$

where ΔE_T is the trap binding energy, which in this case is furnished by analysis of the plastic zone. As per previous continuum studies of H trapping by dislocations [7–10], a characteristic binding energy of 60 kJ/mol [20] was assumed. In actuality,

Table 1
Thermo-mechanical parameters of the rolling contact simulation.

	20 °C	100 °C
Elastic modulus (GPa)	212	207
Specific heat capacity (J/kg K)	461	479
Thermal conductivity (W/m K)	39.6	41.6
Thermal expansion coefficient (K^{-1})	–	12.1×10^{-6}