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Numerical investigation of fatigue strength of grain size gradient materials under heterogeneous stress states in a notched specimen

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ABSTRACT

A possible consequence of forging in common steels is the apparition of a grain size gradient in the width of the component. For railway axles in service, this microstructure gradient is superimposed to the stress gradient introduced by the external load of rotatory bending imposed on the axle. To investigate the combined effects of these gradients on the fatigue lifetime of a forged railway axle, a numerical investigation of the effects of microstructure gradients inserted in a notched specimen is proposed, with respect to different fatigue indicators. In particular, the predictions of an approach based on the theory of critical distances seem to be very promising in this case.

1. Introduction

Ever since the Paris-Versailles accident in the 1840's, railway axles have been a major concern for researchers in the field of fatigue. Due to their loading in rotatory bending, which is in general superimposed in the most critical areas to a local stress gradient induced by notches, they are a typical application of fatigue in the presence of gradients. In the case of forged axles, the macroscopic stress gradients resulting from the external load can be superimposed to microstructural ones, for instance varying grain size in the width of the axle.

Even in the more common case of a homogeneous microstructure, the design of such mechanical parts remains an open problem, as to the authors' best knowledge, there is currently no fatigue criterion that predicts these combined effects in a satisfactory manner. In fact, some of the most frequently used fatigue criteria employed for the design of structures undergoing multiaxial loadings, such as Dang Van's [1] and Crossland's [2] criteria, fail to accurately account for such gradients effects. A wide range of approaches have been attempted to deal with this issue. Papadopoulos et al. [3] proposed a non local-formulation of the Crossland criterion, introducing the gradient of the hydrostatic pressure. This approach was later extended to other criteria by Norberg and co-workers [4], who underlined, in their case, the better predictability associated with probabilistic approaches. These approaches, built on a weakest link framework [5–7] have gained in popularity, thanks to excellent failure predictions with respect to experiment.

The success of such approaches stems from their capacity to address the random nature of the fatigue phenomenon. From a physical perspective, this randomness is a direct result of heterogeneities present at the microstructure scale (e.g. grain disorientations, inclusions, grain boundaries, defects). However, in most probabilistic approaches this aspect is often masked in macro-scale distributions of fatigue probabilities. In recent years, the emergence of constitutive laws taking into account physical deformation mechanisms at the grain scale ([8,9], for instance) has led to the development of an alternative approach: the statistical study of the fatigue response of polycrystalline aggregates, with respect to some fatigue indicator parameters (FIPs), as introduced by [10] (see [11] for a review). In the case of gradient fatigue, this approach has shown promising results: Bertolino et al. [12] have associated the limitations of Dang Van's criterion with the limited number of grains actually undergoing critical stress in the case of gradient fatigue, and [13] have proposed a statistically defined, microstructure sensitive fatigue notch factor based on numerous aggregates simulations.

The latter category seems entirely indicated to deal with the combined issues of gradient fatigue and heterogeneous underlying

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microstructure, for instance in the case of grain size gradients. For steels, grain size can play an important role in the fatigue life. Some authors [14,15] have found that the fatigue limit could be significantly higher for smaller grain sizes, which they imputed to hardening mechanisms similar to those encountered in monotonic cases. Therefore, to efficiently tackle size effects, the constitutive laws used at the grain scale must be able to reflect hardening mechanisms related to grain size. The crystal plasticity constitutive laws encountered in literature can be divided in two categories: the so-called *phenomenological* approach, based on Cailletaud's [8] work and resting on heuristically defined hardening parameters, and the so-called *physically based* approach [9], which hardening mechanisms are governed by the evolution of parameters such as dislocation densities. The first category is predominant in fatigue studies, and has accumulated significant results, such as the relative importance of elastic anisotropy and crystal plasticity on FIP distributions [16,17], or the importance of local grain cluster effects [18] on individual grain responses. The second category is less encountered in fatigue applications, due to a more difficult identification of the constitutive parameters. Sweeney and coworkers [19] however recently emphasized the relation between local dislocation densities predicted by simulations and experimentally observed crack nucleation on iron oligo-crystals.

Nevertheless, accounting for size effects in a physically consistent manner requires to extend these formulations to non-local descriptions, at a tremendous computational cost. To this day, this approach is mostly limited to simplified microstructures with reduced number of grains [20]. In the case where a macroscopic stress gradient is superimposed to a grain size gradient, over the same characteristic length scale (i.e. covering several hundreds/thousands grains for usual grain sizes, which is the case in a forged railway axle), implementing such non-local constitutive laws remains challenging. The present study aims to circumvent this difficulty by modeling the micro plasticity and hardening mechanisms occurring at the grain scale in a qualitative manner. The proposed approach is to describe individual grain behavior by macroscopic von Mises plasticity models taking the grain size into account to qualitatively reflect grain size effects. This simplification, further discussed in the following sections, seems acceptable if the number of grains involved is sufficiently important.

The present paper is an attempt at characterizing the impact of grain size gradients on the fatigue response of a component subjected to a macroscopic stress gradient. First, a numerical model of this configuration, implementing microstructure gradients on a simplified, axle-representative specimen is proposed. A set of FIPs is then chosen to evaluate the impact of three different microstructure gradients on the fatigue response of the specimen. The relative relevance of these FIPs is then discussed in the final section, and general conclusions on the impact of the microstructures are drawn. In particular, a criterion based on Taylor's theory of critical distances [21] is proposed and reviewed through the prism of aggregate calculations.

2. Numerical model

2.1. Model geometry and mesh

In order to qualitatively assess the mechanical response of polycrystalline aggregates under macroscopical stress gradients, a solution is to place the microstructural gradients at the root of a notched specimen. For a forged axle steel, the microstructural gradient support length is typically the whole width of the component, that is to say, the same support length as the stress gradient. The chosen geometry is then a two-scale model, consisting of a 1 mm × 1 mm patch, inserted at the root of a notched specimen (Fig. 1). The model is two dimensional, and the plane strain formalism is adopted. The notch geometry, determined by the $\frac{r}{d}$ and $\frac{D}{d}$ ratios, is chosen to reproduce the stress concentration observed on an average railway axle at the fillet joining the wheel seat and the axle body (the previous ratios are identical for the axle and the chosen geometry). On the notched specimen, r is the notch radius, D the width of the specimen, and d the depth of the notch (see Fig. 1). In practice, D is arbitrarily set to 50 mm, and r and d values are deduced from the axle body diameter, wheel seat diameter and fillet radius. For consistency with typical grain sizes encountered in railway steels (about 25 μm), a realistic patch typically contains around 1500 grains.

In practice, the geometry of the specimen is generated extensively with the SALOME Meca software [22], and the aggregate geometry is generated using the Neper software [23]. The resulting multi-scale geometry is then meshed using the netgen algorithm. An example of a mesh produced by this procedure is presented in Fig. 1, with a reduced amount of grains for illustration. The mesh consists of linear triangular elements. For representative aggregates (1500–2000 grains), the mesh contains approximately 150 000 elements. Displacement boundary conditions are imposed on the upper and lower surfaces.

This study is limited to two dimensional microstructures. Such aggregates present limitations in the representation of actual microstructures, because at the exception of thin film coatings, in most materials out of plane grain interaction have to be taken into account to model a realistic behavior. Comparison of the surface response of 3D aggregates for different internal grain geometries [24] have shown, however, that the surface strain response is only slightly affected by the underlying microstructure. When considering averaged strain values per grain, the difference is found to be negligible. As the goal here is not so much to try and confirm experimental measurements as to draw general conclusions on the aggregate behavior, limiting the study to 2D aggregates and averaged quantities per grain seems an acceptable compromise.

2.2. Polycrystalline aggregates generation

A common tool of generating virtual microstructures is the use of Voronoi polyhedra, or Voronoi tessellations [25]. Such a tessellation fills the space with no overlaps and no gaps, similarly to a real microstructure. Furthermore, for randomly distributed seeds, the resulting grain size distribution typically exhibits a normal behavior, which is frequently encountered on EBSD (electron backscatter diffraction) cartographies of metallic microstructures [26]. In the case of the axle steel, as a first approximation this kind of tessellation is used.

Voronoi tessellations being completely determined by the position of a given set of seeds, they offer a very easy way to create microstructural gradients. A simple method is to assign each region of the polycrystalline patch a chosen seed density, and to distribute seeds randomly in each region according to this density parameter. It is a simple and convenient way of controlling local grain size while conserving the random geometries associated to Poisson-Voronoi tessellations, and realistic grain geometries.

The chosen approach to distribute seeds can be summed up in three steps:

1. Subdivide the 1 mm × 1 mm patch in a given number of vertical bands where the local grain size will be homogeneous. Arbitrarily, 10 regions are thus defined (defining 100 μm × 1 mm bands, regions significant enough in surface with respect to the average grain size of the considered steels, 30–50 μm).
2. Set a given seed density for each region.
3. Distribute seeds randomly in each region according to the previously determined seed density.