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Multi-scale investigation of various gradient effects in fatigue

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Résumé — This study aims at characterizing the influence of gradients at different scales (geometry, microstructure, mechanical properties) on fatigue strength through a multi-scale finite element modelling associated to the Crossland high cycle fatigue criterion.

Mots clés — Cristal plasticity, Critical distance, Multiaxial fatigue, Gradient effect

1 Introduction

Gradient-effect is a well known phenomenon in fatigue, accounting for the fact that structures undergoing a non-uniform load generally exhibit a longer fatigue lifetime than a structure uniformly loaded at the same maximum load. In the case of railway axles fatigue lifetime estimation, a consistent fatigue criterion has to take into account the fact that the axles is subjected to a global stress gradient as it undergoes rotating bending, superimposed in the most critical zones to a local geometrical stress concentration due to the presence of notches. These macroscopic gradients can also be superimposed to microstructural ones coming from mechanical properties gradients associated to surface treatments or manufacturing processes.

In fact some of the most popular fatigue criteria used for the design of structures undergoing multi-axial loadings (such as Dang Van's and Crossland's criteria) fail to accurately account for such gradients effects. Dang Van, for instance, assumes that the number of grains in the representative elementary volume (R.E.V.) is important enough to consider that all crystallographic orientations can be found in the R.E.V., and therefore there will be at least one grain that is in the most critical orientation with respect to the global load. In many cases this assumption remains valid. However, in the case of notched components, the volume in which fatigue mechanisms actually occur can be very limited relatively to the specimen size, and it has been shown [1] that this assumption can lead to a significant underestimation of the specimen lifetime.

To overcome this limitation, several propositions have been made, either by extending existing criteria to non-local expressions [2] or following radically new approaches such as the theory of critical distances [3]. This theory assumes the existence of critical distance d , function of the material, and corresponding to the distance from the notch tip where fatigue criteria should be evaluated to produce correct lifetime estimations for notched specimen. However, to this day there is no satisfactory physical explanation to the good results of the critical distance theory. The present study aims to evaluate the behaviour of a classical multiaxial fatigue criterion evaluated at the grain scale in a polycrystalline aggregate located in the notch tip of a plane specimen, thus allowing general considerations regarding the aggregate behaviour with respect to explicit material parameters such as grain size and orientation. In an attempt to evaluate how grain size impacts the fatigue behaviour of the aggregate, several aggregates with varying grain size distributions are tested. As a first approximation, crystalline laws are not used, for simplicity the global material law is modified within each grain to account for its size and orientation. Explicit microstructure comprehension is also a way to link grain size and orientation to the critical distances theory's conclusions.

2 Numerical model and hypothesis

2.1 Polycrystalline aggregate generation

Several methods of polycrystalline aggregates generation can be found in literature. In [4], a method for running finite element simulations on a multi-scale specimen designed from an EBSD cartography is detailed. This method implies regular meshing of grain geometries, the main drawback being that grain boundary geometry is badly represented. The most common mean of generating virtual microstructures is the use of Voronoi polyhedra, or Voronoi tessellations.

Let $E = \{G_i(x_i)\}$ be a set of points taken in a spatial domain $D \in \mathfrak{R}^n$ and $d(\bullet, \bullet)$ a norm, every point G_i can be associated to a Voronoi polyhedron as follows :

$$C_i = \{P(\underline{x}) \in D | d(P, G_i) < d(P, G_j) \quad \forall j \neq i\} \quad (1)$$

i.e, a Voronoi cell C_i associated with a site $G_i(x_i)$ is the set of points that lie closer to G_i than to any other point of E , with respect to the norm d . A Voronoi tessellation is therefore entirely determined by the distribution of its site coordinates. Such a tessellation fills the space with no overlaps and no gaps, similarly to a metallic microstructure. The Voronoi tessellation associated to a random distribution of points is called a Poisson-Voronoi (PV) tessellation. In the case of the axle steel (EA1N) microstructure, as a first approximation this kind of tessellation is used fig. 1. The geometry of the tessellations strongly depends on the norm being used, however for simplicity only the euclidean norm has been used in this work.

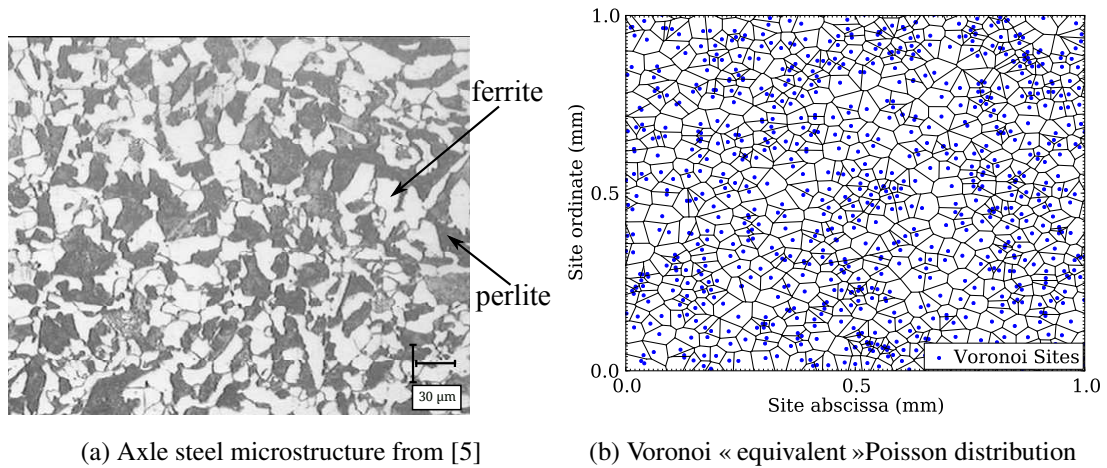


Fig. 1 – Grain distribution modelling

This study is also limited to two dimensionnal Voronoi tessellations. Such aggregates are not representative of actual microstructure, because a the exception of thin film coatings, in most materials out of plane grain interaction have to be taken into account to model a realistic behaviour. However, the study of a 3D aggregate presents several drawbacks : the results are harder to interpret, and the calculation time is drastically increased. As the goal here is not so much to try and confirm experimental measurements as to draw general conclusions on the aggregate behaviour, this is not so much of a setback. The finite element model implementing Voronoi patches is detailed in the next section.

2.2 Finite element model and hypothesis

In the future, an experimental campaign will be carried out on notched specimens, the geometry of which has been determined so that the local stress concentration factor is similar to the one present in railway axles notches. The numerical model consists of this geometry into which a 1mmx1mm patch containing the aggregate is inserted at the root of the notch. To be consistent with the axle steel microstructure, the mean grain size in the aggregate should be around 30-50µm.

In practice, the geometry of the specimen is generated extensively with the SALOME Meca software, and the aggregate geometry is generated using the neper software [6]. As neper only generates 3D aggre-

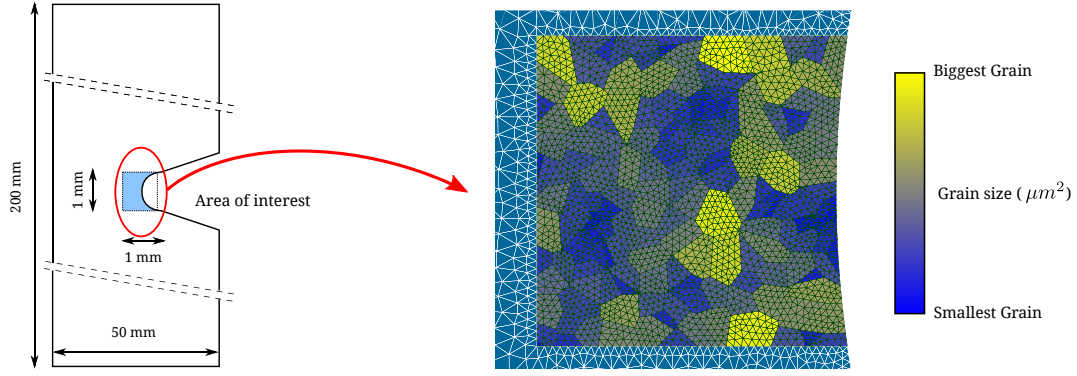


Fig. 2 – Multi-scale model and geometry

gates, the resulting geometry is post-treated using python routines. The resulting multi-scale geometry is then meshed using the netgen algorithm.

An example a mesh produced by this procedure is presented in fig. 2, with a small amount of grains (≈ 200). The mesh consists of 2D, linear tetra-elements, and as experimental tests will include four-point bending on rather large specimens, the plane strain formalism is used. For representative aggregates (≈ 2000 grains), the mesh contains approximately 150 000 elements.

2.3 Material macroscopic behaviour

Previous works on the axle steel (EA1N) [5] have shown that a law combining isotropic and kinematic hardening, as described in [7] reflects satisfyingly the cyclic behaviour of the material. This law is summarized through equations [2-5] :

$$\dot{\epsilon}^p = \epsilon_{eq}^p \frac{\partial f}{\partial \sigma} \quad (2)$$

$$f = J_2(\sigma - X) - R - \sigma_y \leq 0 \quad (3)$$

$$\dot{R} = b(R_\infty - R)\dot{p} \quad (4)$$

$$\dot{X} = \frac{2}{3}C\dot{\epsilon}^p - \gamma X\dot{p} \quad (5)$$

The evolution of the elastic domain is governed by the combined evolutions of the thermodynamic force R and the kinematic hardening variable X . This results effectively in a translation and a uniform expansion of the original domain. In addition to the elastic parameters E and ν , five parameters are necessary to implement it in a finite element solver : $\{\sigma_y, R_\infty, b, C, \gamma\}$

σ_y is the initial value of R , R_∞ is its asymptotic value, and b illustrates the speed with which R reaches its final value. These parameters are those identified by [5] using the SiDolo software. This law is affected to all the mesh elements that are outside the patch containing the aggregate.

2.4 Material mesoscopic modelisation

To account for the microstructural heterogeneities at the grain scale, as a first approximation, it is possible to assign each grain a slightly modified Lemaitre & Chaboche type law, into which the yield strength σ_y becomes a function of grain size d , through the so-called Hall-Petch law (eq. 6) :

$$\sigma_y = \sigma_0 + \frac{k_y}{\sqrt{d}} \quad (6)$$

where σ_0 and k_y are material constants. These parameters were chosen so that, for a Poisson Voronoi tessellation whose resulting grain size distribution was comparable to that of the original material, the

mean yield strength of the distribution given by eq.6 and the axle steel (EA1N) yield strength coincided. The obtained parameters are consistent with those found in literature for a similar steel.

To model grain orientation, a further step is to alter the previously obtained "theoretical" distribution, by drawing the final yield strength in the random sampling from the normal distribution $N(\sigma_y, \mu)$ where σ_y is obtained through eq 6. μ is chosen according to the results of [4].

The different steps are summarised on fig. 3 :

- fig. 3a shows the initial grain size distribution
- fig. 3b shows the yield strength values obtained for that distribution through eq. 6
- fig. 3c shows the final yield strength distribution

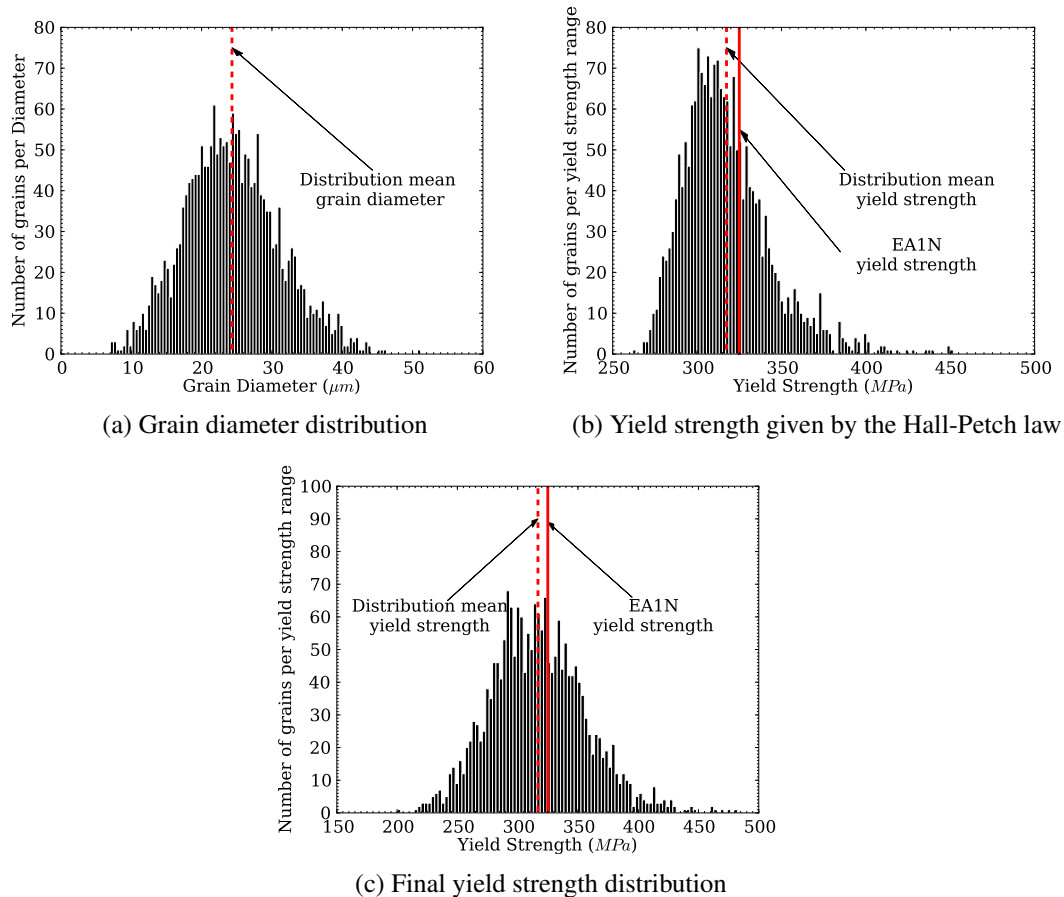


Fig. 3 – Grain distribution building steps

2.5 Validation of the mesoscopic model

In the previous paragraph, it has been assumed that a distribution of yield strength whose mean value is roughly the same as that of the axle steel would describe correctly the material response in the notch area. To validate this assumption, a simple simulation is run : a patch of approximately 200 grains is inserted in a plain sample, and the aggregate homogenised response is compared to the global material reaction under the same load. The results of this simulation are presented on fig. 4.

The dotted curve presents the macroscopic behaviour, and each coloured line presents the axial stress response of a grain. It is clear that the mean behaviour of the aggregate is very similar to that of the original material. The zoom over the yield stress area also reflects the strong heterogeneities arising in the aggregate when some grain enter the plastic domain and other keep an elastic response. This simulations tends to support the assumptions made regarding the distribution of yield strengths.

2.6 Methodology

At this stage, we have defined the following :

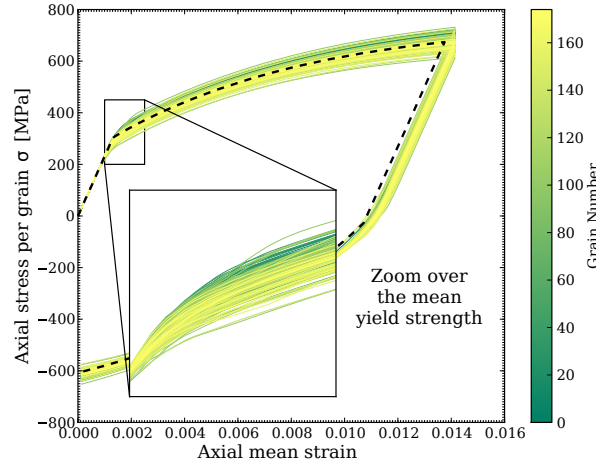


Fig. 4 – Overall material behaviour compared with the mechanical behaviour of each grain

- A pattern to generate physically relevant microstructures
- A macroscopical geometry in which the aggregates will be inserted
- A model linking grain size and material behaviour at the grain scale

In the rest of the present study, we will be focusing on the influence of the microstructural properties in the notch root on a classical fatigue criterion. To do so, the following methodology has been followed : the macroscopic geometry of the bi-scale model is left unchanged, the loading path corresponds to that of a tensile test, the intensity of which is sufficient to cause mesoplasticity in the aggregate, but low enough to keep the overall material behaviour in the elastic domain. Those parameters being fixed, three aggregates are generated through the procedure depicted in paragraph 2.2, but each with a different grain size gradient between the interior and the free surface of the specimen (fig.5). The outer grains are chosen smaller to reflect a manufacturing process similar to quenching. Then, a cyclic tensile test with a load ratio $R = -1$ is simulated. The global load is tension, superimposed to a local stress gradient in the notch vicinity. The Crossland criterion, used to discriminate the different results, is described in the next section.

2.7 The Crossland criterion

To evaluate the comparative criticality of each aggregate, the Crossland criterion is chosen arbitrarily. This criterion takes into account the magnitude of the octahedral shear stress $\sqrt{J_{2a}}$ and the maximum hydrostatic stress $P_{h,max}$ encountered during the load :

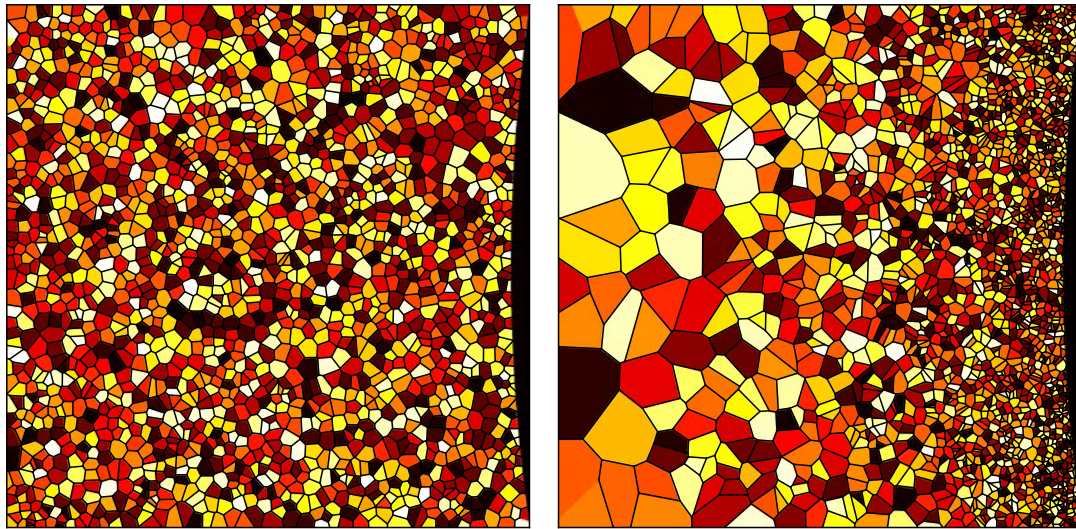
$$\sqrt{J_{2,a}} + \alpha P_{h,max} \leq \beta \quad (7)$$

The two coefficients α and β are obtained through fully reversed tensile and torsional fatigue tests :

$$\alpha = \frac{t_{-1} - \frac{s_{-1}}{\sqrt{3}}}{\frac{s_{-1}}{3}}, \beta = t_{-1} \quad (8)$$

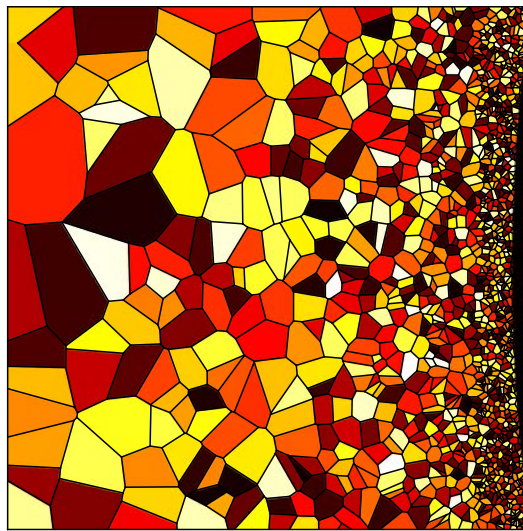
where t_{-1} and s_{-1} are respectively the fully reversed tensile and torsional limits. $J_{2,a}$ is the radius of the smallest hypersphere circumscribing the loading path in the deviatoric space associated with the tensor σ :

$$\sqrt{J_{2,a}} = \frac{1}{2\sqrt{2}} \max_{t_1} \left\{ \max_{t_2} \sqrt{[s(t_2) - s(t_1)] : [s(t_2) - s(t_1)]} \right\} \quad (9)$$



(a) Aggregate 1

(b) Aggregate 2



(c) Aggregate 3

Fig. 5 – 1x1mm Aggregates

3 Results

Figure 6 summarises the simulations results. The axial stress in each grain is plotted for the three aggregates in fig. [6a-6c]. The values correspond to the maximum axial stress encountered in the stabilised cycle. At this point, heterogeneities are clearly visible within the aggregate. Also, and in spite of the significant grain difference in grain size (i.e. yield strength) at the notch tip, the stress ranges within the three aggregates are of the same order of magnitude. This is consistent with an overall elastic behaviour hypothesis.

As illustrated on fig. [6d-6f], the values of the Crossland criterion are noticeably higher than the material fatigue limit of the considered steel, in all three cases. This is not so much of a setback, as what we are focusing on is rather the comparative behaviour of the Crossland criterion on the three aggregates. It is clear, that although the most critical points of every simulations lie close to each other, the scatter tendency varies significantly between the three aggregates. In the case of the homogeneous grain size/ yield strength distribution, the scatter intensity increases gradually with the notch proximity. The apparition of scatter in the criterion is linked to the apparition of plasticity within the grains bordering the notch area. If the whole aggregate had remained in the elastic domain, the computation would have yielded a straight line, independently of the grain size. When a size gradient is present, however, the scatter intensity does not follow the same pattern. A certain scatter is observable at first, but it decreases

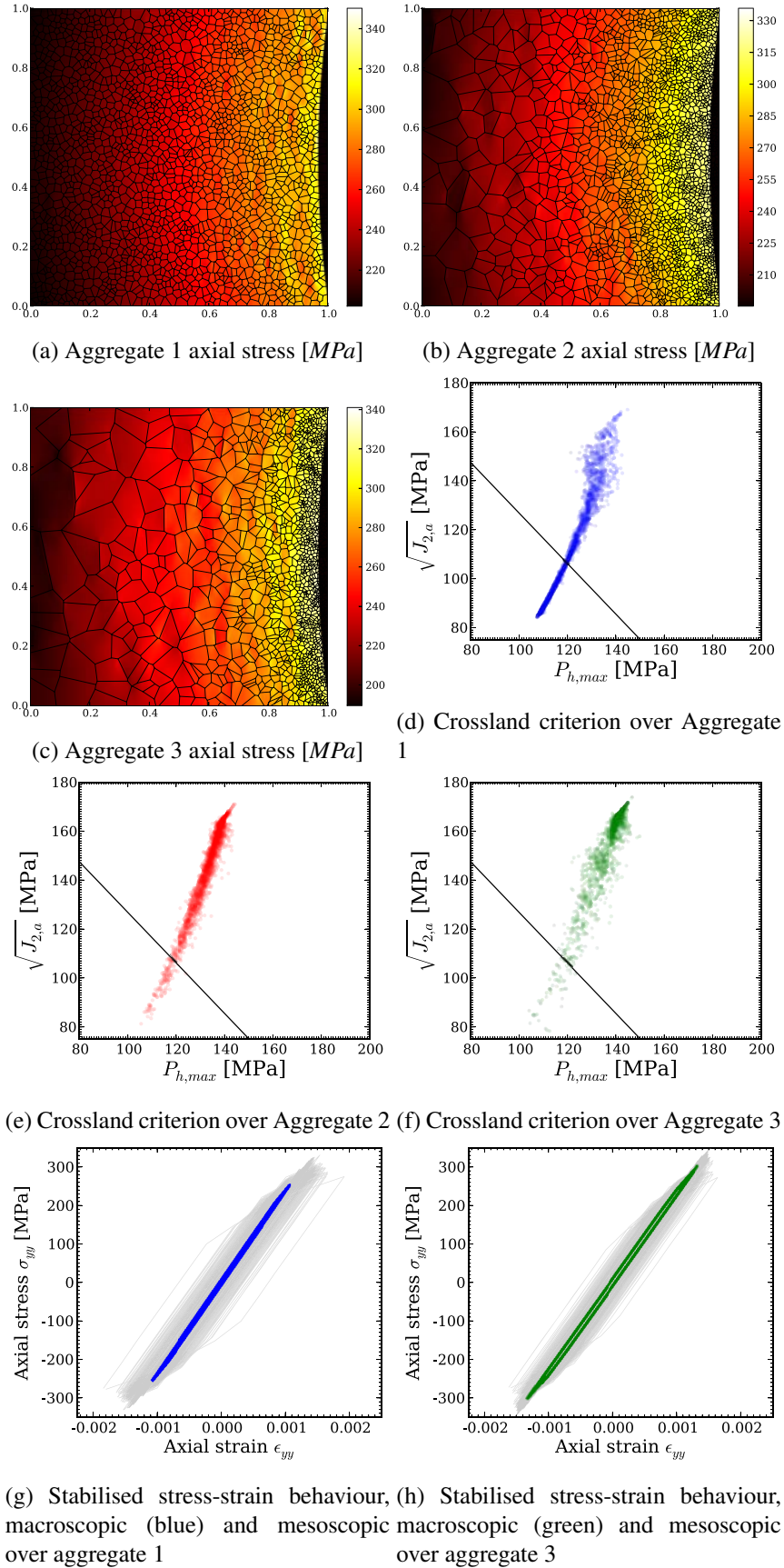


Fig. 6 – Numerical results

in the vicinity of the notch root, for the most critical values of the Crossland criterion. This phenomenon is even more observable for the « smooth » gradient aggregate, where the smallest grain are more numerous. This can be explained through the following considerations, as we get near the notch tip, two things occur :

- 1 The average stress increases
- 2 The average yield strength increases even faster

As a result, the behaviour of the most critically located grains become elastic at the notch root, which is confirmed by the stabilised stress/strain cycles plotted on fig.[6g-6h]. This result is interesting, because it can be linked to experimental observations where crack initiation occur under the surface of the specimen, and this is in accordance to with the principle of the theory of critical distances. In the case of a homogeneous aggregate, the scatter is important from a certain distance to the notch tip on, therefore it is also possible that fatigue can initiate in many grains, and not necessarily the most critically located one.

The final point of discussion regards the values taken by the Crossland criterion, in the case of material exhibiting a gradient of mechanical properties. It is clear that a higher value of the criterion does not necessarily mean a higher failure probability as illustrated on the stabilised stress/strain curves on fig.[6g-6h]. The Crossland criterion is based on the extremal stress values of this circle, which is not pertinent in the case of a gradient properties material :

- 1 The fatigue limit of the material does not bear much sense, since the inner and outer grains have significantly different behaviours
- 2 Several infinite lifetime lines should be used to reflect this.
- 2 Higher stress does not necessary mean the apparition of grain plasticity

In fact a physically consistent criterion should be able to distinguish the grains exhibiting a plastic accommodated behaviour from the ones experiencing elastic shakedown. Indeed, a grain storing energy cycle after cycle is likely to initiate a fatigue crack, whereas a better oriented grain sustaining the same stress will not be a threat to the structure integrity. In future works, low cycle fatigue tests will be carried out on a quenched specimen to see if the results corroborate the previous conclusions.

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