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Micromechanical local approach to brittle failure in bainite high resolution polycrystals: a short presentation

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Abstract

The problem of determining the probability of failure in a brittle material from a micromechanical local approach has recently been addressed in few works ([3; 4; 2]), all related to bainite polycrystals at different temperatures and states of irradiation. They have separately paved the ground for a full-field modelling with high realism in terms of constitutive modelling and microstructural morphology. This work first contributes to enhance this realism by assembling the most pertinent/valuable characteristics (dislocation density based model, large deformation framework, fully controlled triaxiality conditions, explicit microstructure representation of grains and sub-grains, ...) and by accounting for a statistically representative Volume Element; this condition indeed must be fulfilled in order to capture rare events like brittle micro-fractures which, in the stress analysis, correspond to the tails of distribution curves. The second original contribution of this work concerns the methodology for determining fracture probabilities: rather than classically –and abruptly– considering a polycrystal as broken as soon as an elementary link (grain or sub-grain) has failed, the possibility of microcrack arrest at microstructural barriers is introduced, which enables to determine the probability of polycrystal failure according to different scenarii of multiple micro-fractures.

Key words: Brittle failure, Micromechanical local approach, Polycrystals, Microstructural barriers

1. Introduction

Low alloy bainitic steels are widely used in nuclear industry. A comprehensive and reliable prediction of their resistance and life-time has to account for the corresponding conditions of service: a wide range of temperatures combined with the exposure to neutron radiation. The temperature acts on the dislocation mechanisms which take

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place for accommodating stresses whereas radiation causes the formation of defects (interstitial loops, void clusters and precipitates). One has thus to face with the problem of interacting dislocations and defects within a highly heterogeneous crystalline material for predicting hardening and embrittlement which are directly related to failure probability.

Following several developments of microstructure and dislocation density based models dedicated to the plastic behaviour and brittle failure of low carbon bainitic steels [3; 4; 2], the present work (after [9]) proposes to extend the modelling by combining several points that have been already considered: *(i)* microstructures with enhanced realism in terms of crystal orientations, morphology, size and statistical representativity, *(ii)* dislocation density based constitutive laws and *(iii)* large deformation framework.

A full-field approach (section 2) has been applied to the case of bainite polycrystals subjected to particular triaxiality conditions at different temperatures. The resulting deformation and stress fields are post-processed in order to determine probabilities of failure according to a new “micromechanical local approach” (section 3). With this qualification, it is meant that the approach accounts for micromechanical fields (from which microcracks activity can be predicted within either grains or subgrains of the microstructure) for determining the probability of crack propagation within a material element located at the crack tip of a CT specimen. As regards the classical weakest link approach which postulates a straightforward fracture as soon as a sub-domain (grain or sub-grain) is broken, our approach offers the possibility to describe/predict the polycrystal failure according to different scenarios of microfractures, where microcracks can be arrested at microstructural barriers or propagate.

2. Full-field modelling

Low alloy bainitic steels are meant to provide particular mechanical performances over a wide range of temperatures. Their characteristics, as regards other steels, can be related to the high complexity of their microstructure, featuring different phases (cementite, ferrite) and entities (precipitates, laths, packets, grains...) at different scales. For the sake of accurately modelling local interactions between these entities, which are at the origin of high local cleavage stresses, the analyses performed in [2; 3] have allowed to establish the main characteristics of the microstructure that have to be accounted for: an explicit representation of primary austenite grains and bainite packets within each primary grain, a mean representation of the laths constituted by a homogeneous mixture of ferrite laths and cementite precipitates (which is justified by the fact that misorientations between laths of a same packet are small), and a random distribution of carbides within packets which are considered for determining local fracture probabilities. Furthermore, the crystallographic orientations of the bainite packets have to respect relationships of the type Kurdjumov-Sachs (KW) or Nishiyama-Wassermann (NW) *w.r.t.* primary austenite grains orientations. It has also been observed ▶▶ in [1; 2]◀◀ that the determination of packet-to-packet local interactions were particularly mesh sensitive and that consequently, packets interfaces should *(i)* be flat for the sake of realism and *(ii)* strictly conform elements boundaries in order to exclude discretization effects.

In the continuation of previous works ([3; 4; 2]), this study addresses the problem of failure probability in a Volume Element (VE) which has to be representative

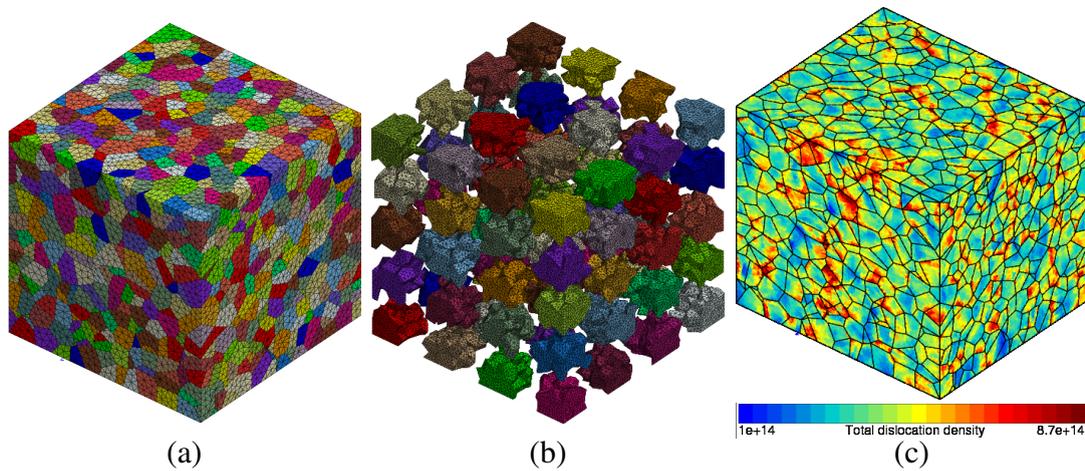


Figure 1: Unstructured mesh of a 4096-cell Voronoi mosaic representing a bainite polycrystal: 670000 nodes, 500000 ten-node tetrahedral elements, 27 sub-domains for parallel computations. (a) each Voronoi cell is a bainite packet; (b) exploded view of the primary austenitic grains, constituted by 50 packets on average; (c) contour plot of the total dislocation density for 10% plane strain tension.

morphologically as well as statistically. Prevailing to this latter condition, both the number of primary austenite grains and the mean number of packets per grain must be large enough. Here, 50 packets per grain -in average- and 80 primary grains have been used. ►► This largely ensures the representativity of the polycrystal *w.r.t.* effective properties or mean responses per packet in a bulk polycrystal. Concerning packet orientations and boundary misorientations, which are respectively involved in cleavage fracture occurrences and microcrack deviations or arrests at packet boundaries [5], the statistical representativity remains tentative at this state of the study. Supplementary analyses on other realisations of polycrystals or on a larger polycrystal would bring out answers on this issue.◀◀ As shown in fig. 1, it has been chosen to model packets with cells of a Voronoi mosaic (4096 cells presently). Cells are then assembled to form primary austenite grains. The software package Neper [10] is used for generating the microstructure and the unstructured mesh ►► (ten-node tetrahedral elements)◀◀, with particular care about the quality of the elements and the refinement around interfaces.

This study aims at predicting the probability of failure of a BCC material at different temperatures and should thus account for the principal mechanisms involved in such materials: thermally activated dislocations, double kink formation, preferential activation of such or such slip system family ($\langle 110 \rangle \{111\}$ or $\langle 112 \rangle \{111\}$). The chosen constitutive laws, inspired from the works of Kocks, Rauch and Tabourot, result from the combination of different models which has been presented in [4; 9]: the temperature dependent flow rule (eq. 1) describes the slip on each slip system through an activation energy depending on the shear stress; the hardening rule on a slip system (eq. 2) is deduced from its dislocation density and that of other slip systems; the dislocation density is related to the slip rate, the mean free path and the critical distance of annihilation (eq. 3).

$$\dot{\gamma}^s = \dot{\gamma}_0 \exp \left[-\frac{\Delta G_0}{k_B T} \left(1 - \left(\frac{|\tau_{eff}^s|}{\tau_R} \right)^p \right)^q \right] \text{sign}(\tau^s) \quad (1)$$

$$\tau_{eff} = \tau^s - \tau_0 - \tau_{int}^s \quad ; \quad \tau_{int}^s = \frac{(\mu b)^2 \sum_{u \neq s} a^{su} \rho^u}{\tau^s - \tau_0} \quad (2)$$

$$\dot{\rho}^s = \frac{|\dot{\gamma}^s|}{b} \left(\frac{1}{D_{grain}} + \frac{\sqrt{\sum_{u \neq s} \rho^u}}{K(T)} - g_c(T) \rho^s \right) \quad (3)$$

The equations are written in a finite strain framework with a multiplicative decomposition of the displacement gradient. Simulations are performed on a parallel supercomputer with the software Zset (zset-software.com, MINES ParisTech, ONERA - the French Aerospace Lab, NW Numerics & Modeling, Inc, [11]).

The parameters that could not be set according to physical observations have been identified for different temperatures by comparison to experimental tensile stress-strain curves at large strain (14%). To this purpose, the full parameter space has first been automatically explored by using a simplified FE polycrystal (343 grains, 1 hexahedral element per grain), then, in a second step, parameter identification has been refined with a more representative VE (1000 Voronoi cells, 1 to 50 cells per primary austenite grain, random or KS or NW orientation relationships, unstructured mesh with 75000 tetrahedral elements).

Fig. 1c illustrates the strong heterogeneity of the mechanical fields (here, the total dislocation density) that arises, both from packet to packet and inside packets, within the polycrystal when it is mechanically loaded. For the computation of local probabilities of fracture, the stresses are averaged over each finite element so that the numerical artefact related to pressure spatial oscillation between the Gauss point of a same elements vanishes. The fields used for post-treatments are thus described on the element level.

3. Micromechanical local approach of failure

In the literature, the terminology of “local approach” of failure classically refers to the methods that predict crack propagation from the local analysis of the stress and strain fields at the crack tip of a CT specimen. In our work, the material element which is considered in a classical local approach is a polycrystal whose behavior is described by a “micromechanical” (full-field) constitutive modelling instead of a macroscopical model. Since the basic building brick of the behaviour is a micromechanical model, the new qualifying term will be “micromechanical local approach”. The output of this new approach on the material element provides, on the specimen (or component) scale, data which are valid for the classical (macroscopic) local approach. Additionally, it introduces a physical framework that gives a chance to description of the damage process such as microcracks activity within packets or grains (stop and go at packet boundaries, ...).

One can first take advantage of this method with the weakest link theory since the elementary links can be chosen to be either primary grains, bainite packets or ultimately finite elements. This theory considers the polycrystalline aggregate as a combination of N independent sub-domains (primary grains, packets, ...) in which the fracture of a single sub-domain causes the aggregate failure. With such conditions, the probability of fracture of the aggregate is simply $p = 1 - \prod_{i=1}^N (1 - p_i^{sd})$ where p_i^{sd} is the probability of fracture of a sub-domain i . p_i^{sd} is determined, as in [3; 4; 1], by means of the Griffith

criterion:

$$p_i^{sd} = \int_0^{\infty} p(\sigma_{loc} > \sigma_G) \rho(\sigma_G) d\sigma_G \quad (4)$$

where $p(\sigma_{loc} > \sigma_G)$ is the probability that the local stress be superior to σ_G and $\rho(\sigma_G) d\sigma_G$ is the probability to find σ_G in the range $[\sigma_G, \sigma_G + d\sigma_G]$. σ_G is the Griffith resistance, *i.e.* the critical stress above which cleavage occurs in crystallographic planes $\{001\}$. It is defined in eq. 5 in terms of the fracture energy γ_f , which is required for generating a new crack surface, and of the carbide size a at an integration point, which is set according to a random distribution based on microstructural observations:

$$\sigma_G = \frac{1}{2} \left[\frac{\pi E \gamma_f}{(1 - \nu^2) a} \right]^{1/2} \quad E : \text{Young modulus; } \nu : \text{Poisson coefficient} \quad (5)$$

Alternatively, the assumption of serial fracture prevailing in the weakest link theory can be abandoned by considering that, due to microstructural barriers such as packet or grain boundaries, the fracture of a single domain of the aggregate could be insufficient for causing the whole aggregate fracture, particularly if the broken link is a single packet among tens others within a same primary austenite grain. ►► Such a scenario is justified by the observation of microcracks arrested at highly misoriented packets boundaries [6; 5] and can also be foreseen for explaining the phenomena of unstable crack propagation and arrest in ferritic steels [7; 8].◄◄ To develop this notion of fracture induced by multiple microcracks, let us note p_I^{pac} the probability that I packets and only I be fractured. This probability is obtained from the analysis of the computed stresses (eq. 4). If we introduce $P_{I/gr}$, the probability that the fracture of I packets leads to the fracture of their primary grain j , then the probability of fracture of grain j reads:

$$p_j^{gr} = \sum_{I=1}^{N_{pack}} p_I^{pac} P_{I/gr} \quad \text{where } N_{pack} \text{ is the number of packets in } j \quad (6)$$

As a single primary grain j can reasonably be considered to be at the origin of the aggregate fracture, and assuming further that its probability of fracture p_j^{gr} depends only on the states of its packets, the probability of fracture of the aggregate becomes:

$$p = 1 - \prod_{i=1}^{N_{gr}} (1 - p_j^{gr}) \quad (7)$$

For the application of this approach, values need to be set for $P_{I/gr}$. They should be deduced from microstructural observations. Still, it is possible to make a first analysis with remarkable ►► realistic ◄◄ values. Let us accept, ►► for the convenience of a simple analysis, ◄◄ that $P_{I/gr} = 1$ for $I \geq 4$. Then, as $\sum_{I=0}^{N_{pack}} p_I^{pac} = 1$:

$$p_j^{gr} = 1 - p_0^{pac} - p_1^{pac} \cdot (1 - P_{1/gr}) - p_2^{pac} \cdot (1 - P_{2/gr}) - p_3^{pac} \cdot (1 - P_{3/gr}) \quad (8)$$

Attributing values taken from the set $(0, 0.5, 1)$ to $P_{1/gr}$, $P_{2/gr}$ and $P_{3/gr}$ leads to the conclusion that $P_{1/gr}$ is the parameter that, much more than the others, influences the prediction of fracture of the aggregate. This is illustrated in tab. 3, in the case of a non irradiated material at -90°C , for $\gamma_R = 14\text{Jm}^{-2}$ and at different stages of the plane strain tension with a triaxiality maintained at the value 2.

$P_{1/gr}$	$P_{2/gr}$	$P_{3/gr}$	Equivalent deformation (%)		
			2.5	5.0	7.5
0	0	0	0.0443	0.3062	0.7135
0	0	1	0.0443	0.3112	0.7150
0	1	1	0.0444	0.3260	0.7196
0.5	1	1	0.7041	0.9800	0.9995
1	1	1	0.9184	0.9996	0.9999

Table 1: Probability of failure of the aggregate (non irradiated material at $-90^{\circ}C$, $\gamma_R = 14Jm^{-2}$ (eq. 5), plane strain tension with a triaxiality maintained at the value 2)

4. Conclusion

This paper presents briefly a strategy for predicting fracture in bainite polycrystals at different temperatures and large strains. It is based on the condition that local packet-to-packet interactions be well represented by the constitutive modelling. This imposes to have a high resolution microstructure with high quality element discretization down to the intra-packets scale and to account for the main physical mechanisms involved in plastic straining and localization in BCC materials, namely the evolution of dislocation densities according to activation, annihilation, slip and hardening. Another condition for applying this strategy is the statistical representativity in terms of elementary heterogeneities, whose fractures are responsible for the fracture of the polycrystal. This is indeed required for capturing rare brittle fracture events, who are particularly under the concern of the nuclear industry. This is also required for the scenario of a material whose fracture is caused by multiple micro-fractures encountering microstructural barriers. A methodology has been proposed to address this problem, **▶▶ which can easily be extended to account for more specific micromechanisms involved in cleavage fracture, for example the influence of a microcrack on the probability of fracture in neighbouring packets.**◀◀ All together, the full-field model and the methodology applied for determining fracture probabilities form a new micromechanical local approach of fracture in bainite polycrystals.

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