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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 ([1–3]), 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 abruptably – 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.

1. Introduction

Low alloy bainitic steels are widely used in nuclear industry. A comprehensive and reliable prediction of their resistance and lifetime 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 place for accomodating 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 behavior and brittle failure of low carbon bainitic steels [1–3], the present work (after [4]) 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 propogation 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 subgrain) is broken, our approach offers the possibility to describe/predict the polycrystal failure according to different scenarii of micro-fractures, 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

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chacteristics, as regards other steels, can be related to the high complexity of their microstruture, featuring different phases (cementite, ferrite) and entities (precipitates, laths, packets, grains...) at different scales. For the sake of accuratly modelling local interactions between these entities, which are at the origin of high local cleavage stresses, the analyses performed in [3,1] 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 [5,3] 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 ([1–3]), this study addresses the problem of failure probability in a Volume Element (VE) which has to be representative 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 [6], the statistical representativity remains tentative at this state of the study. Supplementary analyses on other realizations 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 [7] is used for generating the microstructure and the unstructured mesh (10-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 ($\langle 1\,1\,0\rangle\{1\,1\,1\}$ or $\langle 1\,1\,2\rangle\{1\,1\,1\}$). 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 [2,4]: 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)).

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

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

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

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., [8]).

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, 1–50 cells per primary austenite

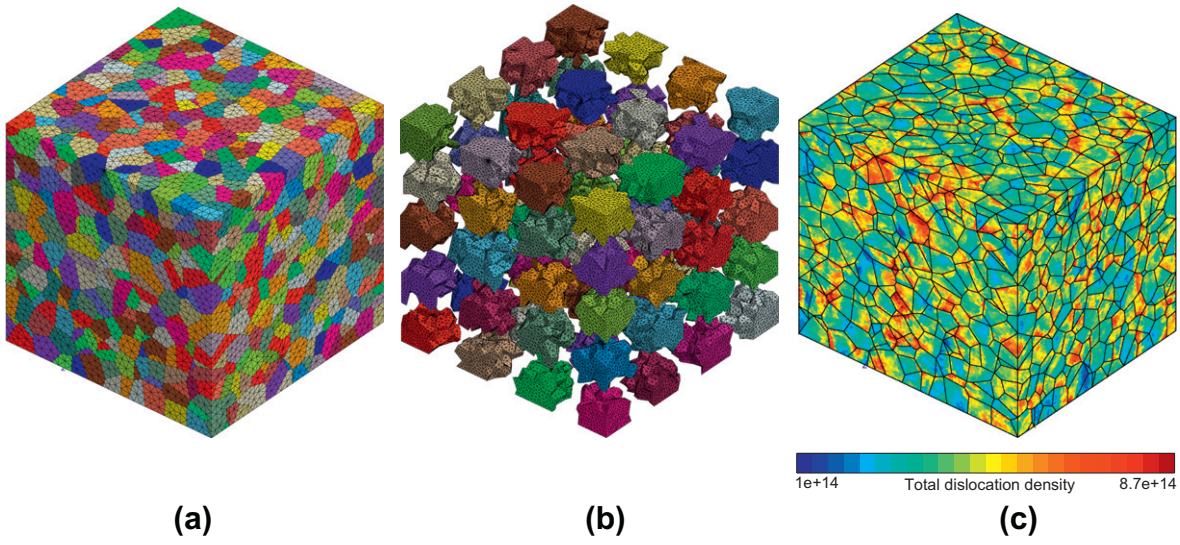

Fig. 1. Unstructured mesh of a 4096-cell Voronoi mosaic representing a bainite polycrystal: 670,000 nodes, 500,000 ten-node tetrahedral elements, 27 sub-domains for parallel computations. (a) Each Voronoi cell is a bainite packet; (b) exploded view of the primary austenitic grains, constituted by 50 packets on average; (c) contour plot of the total dislocation density for 10% plane strain tension.