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Intergranular stress distributions in polycrystalline aggregates of irradiated stainless steel

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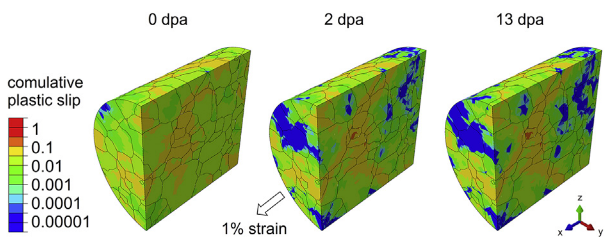
HIGHLIGHTS

- Intergranular normal stress distributions are obtained for irradiated stainless steel.
- Distributions are well approximated by a master curve once rescaled by yield stress.
- A methodology to predict IASCC crack initiation is proposed.

GRAPHICAL ABSTRACT



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ABSTRACT

In order to predict InterGranular Stress Corrosion Cracking (IGSCC) of post-irradiated austenitic stainless steel in Light Water Reactor (LWR) environment, reliable predictions of intergranular stresses are required. Finite elements simulations have been performed on realistic polycrystalline aggregate with recently proposed physically-based crystal plasticity constitutive equations validated for neutron-irradiated austenitic stainless steel. Intergranular normal stress probability density functions are found with respect to plastic strain and irradiation level, for uniaxial loading conditions. In addition, plastic slip activity jumps at grain boundaries are also presented. Intergranular normal stress distributions describe, from a statistical point of view, the potential increase of intergranular stress with respect to the macroscopic stress due to grain-grain interactions. The distributions are shown to be well described by a master curve once rescaled by the macroscopic stress, in the range of irradiation level and strain considered in this study. The upper tail of this master curve is shown to be insensitive to free surface effect, which is relevant for IGSCC predictions, and also relatively insensitive to small perturbations in crystallographic texture, but sensitive to grain shapes.

1. Introduction

Internals structures of Light Water Reactors (LWR) are made mainly of austenitic stainless steels, known for their good mechanical properties such as ductility and toughness, and their resistance to corrosion. Under neutron irradiation, a degradation of these properties is observed, such as a drastic decrease of fracture toughness and a susceptibility to stress corrosion cracking (SCC) [1–3]. This last phenomenon is referring to as Irradiation Assisted Stress Corrosion Cracking (IASCC), as it affects materials under irradiation initially non-sensitive to SCC. IASCC has been observed since the 1980's in both Boiling Water Reactors (BWR) and Pressurized Water Reactors (PWR), with the appearance of intergranular cracks for example in core shrouds in BWRs and baffle-to-former bolts in PWRs [4,5]. Several researches have been

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conducted since then to assess the key parameters affecting both initiation and propagation of intergranular cracks in LWR's environment, parameters than can be divided into three groups: stress level [2,6–9], mechanical behaviour of the material and its chemical composition (which includes initial microstructure and chemical composition, and irradiated defects and segregation [10]), and LWR's environment [11,12].

In recent years, different models have been proposed to predict IASCC of austenitic stainless steels, or more generally InterGranular Stress Corrosion Cracking (IGSCC). In some studies, slip localization, *i.e.* strongly heterogeneous deformation field at the grain scale has been argued to be responsible for IGSCC crack initiation, leading to models based on dislocation pile-up theory or refined slip bands modelling [13]. Other recent studies of SCC cracking are based on simulations of polycrystalline aggregates with cohesive zone models [14], leading to both prediction of initiation and propagation. These models using standard crystal plasticity constitutive equations assume implicitly that rather homogeneous deformation field at the grain scale can be sufficient to assess intergranular cracking. Such models have been used for example to predict SCC of Zircaloy in iodine environment [15] or SCC of cold-worked austenitic steels [16]. These fully coupled models require both an accurate crystal plasticity constitutive law and grain boundaries modelling in order to provide quantitative predictions. As crystal plasticity models are only recently available in the literature for irradiated materials [17,18], and especially irradiated stainless steels [19–21], such simulations have not yet been performed so far for irradiated stainless steel.

These fully coupled models show some drawbacks such as high computational cost due to crack propagation and rather inaccurate intergranular stress prediction due to cohesive zone modelling [22]. Therefore, an intermediate approach is considered here following the work of Diard et al. [23,24], based on the computation of accurate intergranular (normal) stress distributions for irradiated stainless steels for uncracked polycrystalline aggregate, as normal stress at grain boundaries is assumed to be the key parameter for intergranular cracking. Contrary to other studies [23,25] focusing on relations between intergranular stress and orientation of the boundary with respect to the loading direction or to the mismatch of deformations between adjacent grains, full distributions for statistically large number of grains with different orientations are assessed. Combined with an empirical or experimental criterion for grain boundary strength that may depend on oxidation time and irradiation level, such uncoupled modelling could in principle be an efficient tool to predict critical macroscopic stress above which intergranular cracks are expected to be initiated at the grain scale, or number of cracks per unit area. This approach is particularly relevant in the case of SCC of post-irradiated or heavily cold-worked austenitic stainless steel [26] in PWR nominal environment (compared to BWR oxygenated environment), where low propagation rates enable rather weak interactions between intergranular cracks, and thus the appearance of numerous surface cracks, as shown for example in Refs. [10] and [27], for neutron-irradiated and proton-irradiated stainless steel, respectively.

In the first part of the paper, recently proposed crystal plasticity physically-based constitutive equations for neutron-irradiated austenitic stainless steel [20,21] that have been used in this study are described. In a second part, polycrystalline simulations based on a realistic aggregate are presented, leading to the stress distributions at grain boundaries as a function of strain and irradiation level. The effects of free surface, deviations from random crystallographic texture and equiaxed grain shapes are assessed. As a conclusion, and based on these numerical results, a methodology is proposed to obtain a statistical modelling of IGSCC initiation. The range of validity of such modelling is finally discussed.

2. Numerical modelling

2.1. Crystal plasticity constitutive model

A degradation of mechanical properties of irradiated austenitic stainless steels is commonly ascribed to the formation of high density nano-sized irradiation defect clusters, mainly interstitial Frank loops [28], preventing the motion of dislocations thus leading to hardening, and also reducing strain-hardening capabilities. To account for those effects, a crystal plasticity constitutive model developed in Refs. [20,21] is described, with the dislocation and Frank loop density-based evolution laws.

To describe the plastic behaviour of single crystalline material, in general two laws are considered: a shear flow law that activates a slip system and determines its slip rate, and a hardening law that describes the change of slip activation with applied slip by taking into account the evolution of various defects created within the material. The shear flow adopted here for non-irradiated and irradiated conditions is of visco-plastic type and represents isotropic hardening,

$$\dot{\gamma}^{\alpha} = \left\langle \frac{|\tau^{\alpha}| - \tau_c^{\alpha}}{K_0} \right\rangle^{n} \mathrm{sign}(\tau^{\alpha}), \quad \text{with} \quad \langle x \rangle = \begin{cases} x & ; x > 0 \\ 0 & ; x \leq 0 \end{cases} \tag{1}$$

where γ^{α} is shear strain in slip system α (α=1…12 for Face-Centered-Cubic lattice) and τ^{α} and τ_c^{α} are respectively the resolved shear stress and critical resolved shear stress. Parameters K_0 and n regulate the viscosity of the shear flow.

The critical resolved shear stress is additively decomposed into components that contribute to the hardening [29],

$$\tau_c^{\alpha} = \begin{cases} \tau_0 + \mu\sqrt{\sum_{\beta=1}^{12} a^{\alpha\beta} r_D^{\beta}} & ; \text{non} - \text{irradiated} \\ \tau_0 + \tau_a \exp\left(-\frac{|\gamma^{\alpha}|}{\gamma_0}\right) + \mu\sqrt{\sum_{\beta=1}^{12} a^{\alpha\beta} r_D^{\beta}} + \mu\alpha_L\sqrt{\sum_{p=1}^{4} r_L^{p}} & ; \text{irradiated} \end{cases} \tag{2}$$

The hardening law for non-irradiated steels accounts only for dislocation density evolution. Here, r_D^{α} is normalized dislocation density in slip system α (normalization factor b_D^2, with Burgers vector $b_D = 2.54 \times 10^{-10}$ m), τ_0 is lattice friction stress that remains