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# PREDICTION OF GRAIN BOUNDARY STRESS FIELDS INDUCED BY THE IMPINGEMENT OF PERSISTENT SLIP BANDS

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**Abstract**: Persistent slip band (PSB) – Grain boundary (GB) crack initiation is widely observed and documented. Therefore, the prediction of stress fields at PSB-GB interfaces in polycrystals subjected to cyclic deformation is necessary to predict micro-crack initiation. Our FE simulations are based on physically based models, accounting for (i) cubic elasticity and crystal CSS behavior using single crystal data and (ii) production, annihilation, and diffusion of vacancies inducing an increasing free dilatation of PSBs, without using any fitted parameter. We investigate the impact of grain size and PSB width on GB stress fields for both Austenitic stainless Steel and Copper polycrystals. The predicted stress fields will be used to predict the number of cycles to initiate GB micro-cracks.

## Introduction

Cyclic deformation of fcc metals often leads to the creation of slip bands within slabs of grains which remain. These slip bands are called persistent slip bands (PSBs) since they reappear at the same positions after polishing the samples and recycling. PSBs cross the grains and are characterized by their specific extrusion shape through GBs (as shown in Figure 1 below) and free surfaces. The shapes and characteristic lengths of PSBs depend mostly of the considered material, grain size, and orientation of PSBs Burgers vectors [1], [2].

Along lifetime, a certain number of surface cracks are generated. At high and intermediate strain amplitudes and depending on some parameters such as environment, these cracks are mostly transgranular (PSB-matrix) and intergranular (PSB-GB). They are localized at twin boundaries for low strain amplitude. For instance, the majority of micro-cracks are initiated at PSB-GB interfaces for 316L SS in vacuum after 5000 cycles at $\Delta\varepsilon_p/2 = 2.10^{-3}$ [3].

## Context and goals

Some components of the Generation IV nuclear power plant Astrid will be subjected to cyclic deformation in N/Na environment.

As prediction of micro-crack initiation at PSB-matrix interface was treated by [4], we focus here on PSB-GB interface micro-crack initiation. Predicting (i) the deformed shapes of the GBs impacted by PSBs and (ii) the GB stress fields induced by the impingement of PSBs toward GBs is essential to predict micro-crack initiation.

(i) Initially, Essmann et al. [5] proposed a model (EGM I) for the formation and growth of a dynamic extrusion trough migration of vacancies (formed by annihilation of edge dislocations of opposite signs) to the surrounding matrix and channels. Later, Polák [6] developed that model highlighting the effects of diffusion leading to formation of both extrusions (in the center of PSBs) and intrusions (at PSB-matrix interfaces). Then, Polák & Sauzay [7] proposed an analytical model predicting PSB vacancy concentration, migration and extrusion growth rate per cycle depending on material and temperature.

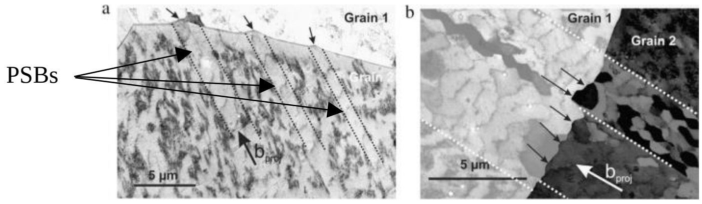

*Figure 1 : (a) (b) ECC images of GB deformations induced by PSBs in cyclically deformed Nickel polycrystals [2].*

(ii) Several studies were conducted in order to predict accurately the GBs stress fields impacted by PSBs. Historically, Liu et al. [9] proposed a physical model based on dislocation accumulation (pile-ups) at PSB-GB interfaces to predict micro-crack initiation. Considering dipole pile-ups, Tanaka & Mura [10] computed GB stress fields by the creation and diffusion of vacancies. Because of their thermoelastic approach, some overestimation of PSB-GB stress fields is expected. By computing stress fields for pile-ups and bands of finite thickness, Sauzay & Vor [11] and Sauzay & Moussa [12] found pile-ups as being

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overestimating the stress fields. Recently, Sauzay & Liu [4] predicted the stress fields and micro-crack initiation at the surface of single crystals induced by vacancy production and annihilation within PSBs and diffusion toward the matrix (our work is based on that latter work). Pile-ups are not considered, the finite element simulation account for finite thickness of PSBs, thermal dilatation and crystal plasticity. In our study we predict both the extrusion height through the GB of a PSB embedded in an elastic matrix with and without a free surface and the stress fields at PSB-GB interface in copper and austenitic stainless steel polycrystals. We study the impact of grain size and PSB width. Different assumptions are adopted:

- Considering only the elastic-plastic behavior of finite thickness PSBs and the elastic matrix.
- Considering only the vacancy production within finite thickness PSBs by imposing a thermal dilatation.
- Considering the synergy of the two latter (more realistic case).

The FE computations are performed accounting for (i) cubic elasticity and crystal CSS behavior using single crystal experiments data [13], (ii) production, annihilation, and diffusion of vacancies inducing a free dilatation within PSBs [4]. A schematic representation of a PSB and its specific characteristic lengths is shown in Figure 2.a. In Figures 2b and 2c are plotted examples of GB displacement and GB normal stress fields (in function of the distance to the grain boundary) due to the impingement of a PSB in copper after producing vacancies during 30.000 cycles (thermal dilatation).

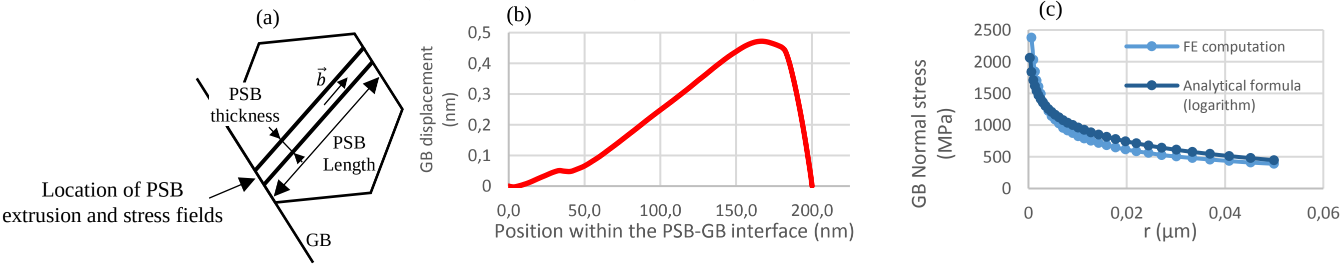

*Figure 2 : (a) Schematic representation of a mesh used for the prediction of the stress field at the PSB-matrix interface; (b), (c) GB displacement and GB normal stress field due to the impingement of a PSB (length : 10µm, thickness : 0,2µm; copper).*

Our next ambition is accounting for the vacancy diffusion toward the surrounding matrix leading to the formation of an intrusion [5], [14] and incorporating a fracture model such as cohesive zone modeling (CZM) or a double criterion using both energy and stress criteria for predicting a number of cycles to initiate GB micro-cracks and compare it with experiments (ours and from the literature).

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