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Introduction to the effect of the screening phenomenon of slip bands within grain microstructure

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Abstract

The aim of the current contribution is to compute grain boundary (GB) stress fields and fracture using respectively finite elements (FE) methods and analytical model in the case of several slip bands (SB) impinging the GB. Indeed, local plasticity in thin bands is largely observed during straining of polycrystals. For instance, channels (or clear bands) within grains are observed after post-irradiation tensile loading [Cui et al, 2013]. Slip bands thickness is about 50 nm which is about hundred times higher than the classical pile-up thickness. The intersection of such slip bands (SBs) with grain boundaries (GBs) can trigger microcracks initiation. Then, it is important to propose a fracture criterion for predicting GB microcracks nucleation as SBs impinge GB. Despite of many issuesdevelop pile-up based models of GB stress fields, observations showthat morethan single slip band are observed in real situation.Then, the main carried out tool is the analysis of the screening effects of SB on parameters of early validated single SB model.

Keywords:Irradiated materials, Finite Fracture Mechanics, Grain boundaries, analytical criteria, strain localization, crystalline plasticity, slip bands interactions, slip bands screening

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1. Introduction

Strain localization is often observed in single and poly-crystals, for instance forming clear bands or persistent slip bands respectively during post-irradiation tensile loading or cyclic loading. This concerns particularly the Faced-Centred Cubic (FCC) metals and alloys subjected to either post-irradiation tensile tests (proton or neutron irradiation with high dose) [Sharp, 1967; Lee et al., 2001; Edwards et al., 2005; Jiao et al., 2005; Byun et al., 2006], cyclic loadings [Lukas et al., 1968; Finney and Laird, 1975; Winter et al., 1981; Mughrabi and Wang, 1988; Man et al., 2002], or even simply tensile loading [Perrin et al., 2010]. Plastic slip is localized in thin slip bands. Their thickness is lower than 1µm but higher than a few ten nm. Usually, slip bands cross all the grains from one grain boundary to the opposite one. Therefore, the slip band length is approximately equal to the grain size which usually varies from a few ten microns to a few hundred microns depending on the material. The degree of slip localization in the thin SBs seems to be high. It could be evaluated using the ratio between the slip band and macroscopic axial plastic strains. Following the AFM (Atomic Force Microscopy) measurements of Jiao et al. [Jiao et al., 2005], this ratio is equal to about 10 for austenitic steels subjected to post-irradiation tensile loading (macroscopic axial strain of 0.03). TEM (Transmission Electronic Microscopy) observations lead to similar evaluations [Sharp, 1967; Edwards et al., 2005]. Such thin SBs are called channels or clear bands. Their thickness is about 50nm. Plastic strain is highly localized in slip bands induced by cyclic loadings as well. Such SBs are often called persistent slip bands (PSBs). Localization degrees, lying between 50 and 100 %, have been measured in PSBs [Winter et al., 1981; Weidner et al., 2006; Weidner et al., 2010]. PSB thickness is about 0.5 µm in Face Centred Cubic (FCC) polycrystals [Mughrabi and Wang, 1988; Man et al., 2002]. Recent 3D Dislocation Dynamics computations, taking into account cross-slip, permitted to predict numerically the formation of slip bands in an austenite crystal [Déprés et al., 2004]. It should be noticed that similar observations of slip localization have been often reported in either body centred cubic (BCC) or hexagonal compact (HCP) metals and alloys. Several computations were carried out for evaluating the plastic slips inside slip bands, particularly in the framework of cycling of ductile metals. Authors first modelled slip bands as elongated inclusions embedded in a matrix which mimics the whole polycrystal [Rasmussen and Pedersen, 1980]. This permitted them to use the analytical solution given by Eshelby for a bulk inclusion. Then, Finite Element computations using crystalline plasticity permitted the investigation of surface effects [Repetto and Ortiz, 1997]. In the case of type B slip bands, that are inclined by 45° with respect to the free surface, both slip magnitude and heterogeneity are considerably enhanced by surface effects [Sauzay et al., 2003], which explains partially the preferential surface fatigue crack initiation. Clear bands and slip bands impinge to grain boundaries. This induces stress or plastic strain concentrations as shown in a copper polycrystal deformed after neutron irradiation of Edwards et al. who observed indeed either local lattice rotations corresponding to high elastic strain concentrations or a considerable amount of (plastic) shearing at the grain boundary if another channel has been nucleated on the opposite side of the grain boundary [Edwards et al., 2005]. Such propagation of a channel in the neighbouring grain was observed [Jiao et al., 2005, Liu et al., 1992], but almost only in the case of singular grain boundaries such as twin boundaries. If no transmission through GBs occurs, then large stress concentrations are induced by the impingement of SBs towards GBs. Recently, high resolution EBSD allowed the measurement of elastic strains at the submicron scale showing the strong stress concentrations induced by slip localization [Ben Britton and Wilkinson, 2012]. Because of these interactions with grain boundaries, clear bands or slip bands are often considered as triggering grain boundary crack initiation and propagation. The corresponding crack initiation mechanism has been investigated experimentally for copper [Liu et al., 1992] and nickel [Lim and Raj, 1984b] polycrystals subjected to cyclic loadings. Concerning grain boundaries, two extreme cases can be considered: On the one hand, general grain boundaries display mostly very high Σ values. That value is defined as the inverse of the fraction of coincident atoms between the two crystallographic networks. Therefore, there is no periodicity along the grain boundary. Their energies as well as their diffusion coefficients are very high. On the other hand, the special boundaries have low Σ values and present generally a periodicity along the grain boundary. Their grain boundary energies as well as their diffusion coefficients are low. The Σ3 twin boundary is a well-known example of special grain boundary. Based on microscopic observations, the authors of the different studies could evaluate which grain boundaries are the most prone to crack initiation and which ones are the less prone to crack initiation. All authors concluded that special boundaries, and particularly Σ3 twin boundaries, are the less prone to stress corrosion cracking (SCC) initiation even if some of them could crack [Alexandreanu and Was, 2003]. It should be noticed that the same result was obtained in copper [Liu et al., 1992] or nickel [Lim and Raj, 1984b] subjected to cyclic deformation carried out in either in air or in inert environment condition. Their low GB energy values lead to high fracture energy and the observed slip band transmission through special GBs decreases GB stress concentrations which is not the case for general GBs. Several modelling approaches focused on the evaluation of grain boundary stress concentrations. Recently, Diard et al. used large-scale Finite Element computations for evaluating stress gradients in the vicinity of grain boundaries, induced by plastic deformation incompatibilities between neighbour grains [Diard et al., 2005]. All these studies highlighted stress concentrations which could promote intergranular crack initiation. Concerning the influence of slip band impingement, GB stress fields have been evaluated analytically using the theory of discrete or continuous dislocation pile-ups. This approach is based on the well-known Stroh model [Stroh, 1957]. The stress singularity induced by an edge or screw pile-up of length $L^{pile\text{-}up}$ is the same as the one of a crack in the framework of linear elastic fracture mechanics (LEFM) [Stroh, 1957]. This length is usually assumed to be close to one-half of the grain size, L. Thanks to the similarity with the LEFM crack problem, the energy release rate, G, may be computed in a straightforward way. As the stress singularity exponent is ½, the application of the Griffith criterion leads to possible microcrack initiation, which is not be true for lower stress exponent values [Leguillon, 2002]. The Griffith criterion is based on the equality between the energy release rate, G, and the GB fracture energy, γ_{fract}. This means that only an energy criterion is required and the crack increment is assumed to be infinitesimal. This modelling has been applied to the prediction of GB microcrack initiation, either in copper polycrystals subjected to cyclic loading [Liu et al., 1992] or pre-irradiated austenitic stainless steels subjected to tensile loading. Applying such modelling to inter-granular crack initiation at the free surface of copper polycrystals subjected to cyclic loading, Liu and co-workers found that the predicted critical remote stress was generally reached when GB microcracks were observed [Liu et al., 1992]. Generally, many cycles are required, which contradicts the conclusions of Liu et al. of instantaneous microcrack initiation provided slip bands exist and stress saturation is reached. Using the pile-up theory as well, Evrard and Sauzay predicted critical remote tensile stresses much lower than the observed ones, whatever the environment [Evrard and Sauzay, 2010]. Therefore, the pile-up theory seems to lead to underestimations of the critical remote stresses when compared to experimental data. Pile-up theories assume that slip is localized on one atomic plane only. But, many experiments and observations show that for many materials and loading conditions, a non-negligible fraction of the slip occurs inside the fatigue slip bands (interferometry measurements [Finney and Laird, 1974], TEM observations [Sauzay et al., 2010] and AFM measurements [Jiao et al., 2005; Weidner et al., 2006 and 2010]). Concerning 316L austenitic stainless steel deformed after pre-irradiation, Byun at al. [Byun et al., 2006] concluded that shear strain is uniformly distributed through the thickness of channels (clear bands). Similar conclusions were drawn by Jiao et al. [Jiao et al., 2005] and Sauzay et al. [Sauzay et al., 2010]. As plastic slip is indeed much more homogeneously distributed than assumed by pile-up theories, these last ones may overestimate the local GB normal stress fields as well as energy release rate values which may lead to the underestimation of the critical remote stress mentioned previously. Taking into account not only the slip band length, L (or pile-up length often assumed to be about one-half of the grain size), but also its thickness, t, may lead to more realistic GB stress fields and improve the microcrack initiation predictions. As mentioned previously, the thickness varies between a few ten nm in pre-irradiated polycrystals to one micron in polycrystals subjected to cyclic loadings. The finite element (FE) method has been used recently in the framework of crystalline elastoplasticity because of the non-linear behaviour of slip bands [Sauzay and Ould Moussa, 2013]. Slip bands of various thickness and lengths were embedded at the free surface of an elastic matrix. The effect of slip band thickness and length as well as remote tensile stress was studied based on the results of numerous FE computations. Analytical formulae describing the GB normal stress singularities induced by slip bands were deduced but only for steels and only particular microstructure geometry. Aiming at studying the effect of slip band screening phenomenon on grain boundary stress fields and fracture, our paper is organized as: The next section is devoted to present the analytical modeling scope and before concluding one section shows the details and results of simulations performed with the cast3m FE software.

2. Theoretical framework

Following Stroh and Griffith works [Stroh, 1967], many issues develop pile-up based models of GB stress fields. However, observations show that the pile-up models underestimate the critical macroscopic stress needed to nucleate GBs microcracks. Such underestimating may be explained by the fact that pile-up stress fields are much higher than slip bands ones. It is worth to highlight that more than one single slip band are observed in plastically deformed grains.

Many parallel slip bands are usually observed even at low plastic strain. Furthermore, depending on plastic slip transmission characteristics through each grain boundary, slip bands in one grain may interact with the neighbor grain ones. Therefore, the current contribution aims at modeling the effect of slip band screening and interactions on GB stress fields and GB fracture. Based on the theory of Matched Limited Expansions [Leguillon and Sanchez, 1987], considering V-notch like close stress fields and crack far stress fields, see Fig. 1.

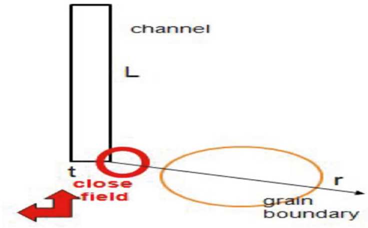

Fig. 1. Sketch of the intersection between one SB and one GB.

The close field expression of the normal GB stress was proposed as:

$$\sigma_n = A_{nn}\sqrt{\frac{L}{t}}\left(\frac{t}{r}\right)^{\alpha}(f\,\Sigma_0 - \tau_0) + \Sigma_n^{\infty} \qquad (1)$$

WhereA_{nn}, L, t, r, f, Σ_0, τ_0 and Σ_n^{∞} are respectively normal GBs stress prefactor, SBs length, SBs thickness, distance along the GBs, Schmid factor, macroscopic applied stress, shear stress yield (in the absence of hardening effect) and the normal GBs stress far from the local zone(Fig. 1).

In addition, the small value of singularity exponent disable us to use the Griffith criterion in the framework of standard fracture mechanics. That is why Finite Fracture Mechanics (FFM) is combined with a double criterion using both energy and stress concepts. This leads to the evaluation of the critical macroscopic stress, given by

$$\Sigma_c = \frac{1}{f}\left[\tau_0 + \left(\frac{2-2\alpha}{C}\right)^{\alpha}(A_{nn})^{2\alpha-1}\sqrt{\frac{t}{L}}\left(\frac{\gamma_{frac}}{t}\right)^{\alpha}\sigma_c^{\,1-2\alpha}\right] \qquad (2)$$

where C is a parameter which outcomes from the computation of the released mechanical energy based on the numerical evolution of a microcrack size increment a, γ_{frac} and σ_c are a model parameter, the fracture energy and stress. According to this model, Σ_c inversely depends on the parameter A_{nn} for a given microstructure geometry and orientations. Indeed, the larger A_{nn}, the smaller Σ_c. It is worth to note that the singularity exponent is less than 0.5.

3. Finite elements (FE) calculations and results

For each considered microstructure, slip bands obeying to crystal plasticity are embedded in a main elastic grain and the surrounding elastic matrix, see Fig. 2.

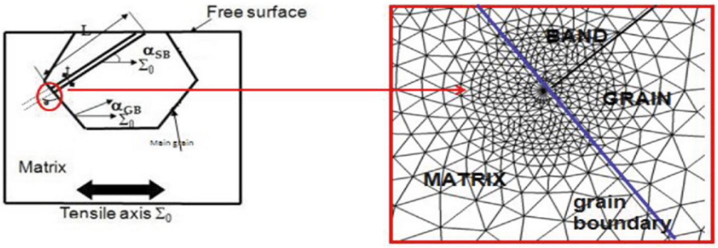

Fig. 2. Sketch of the reference microstructure and the corresponding mesh (zoom)

The present contribution shows quantitative changes in A_{nn} as many SBs expand within the microstructure and impinge the GBs. Indeed, the FE calculations are carried out in different situations, correspond to different microstructures:

- When six parallel bands exist inside the same grain and are regularly spaced (Fig. 3a). The loading conditions are the followings: The macroscopic applied stress Σ_0 is about 393 MPa, the GB orientation is α_{GB} = 35°, the SBs orientation is α_{SB} = 45° and the SB aspect ratio is, $\frac{L}{t}$=100. Fig. 3b shows that A_{nn} decreases along GBs axis, SB after SB, from a value (A_{nn}) which corresponds almost to the case of one isolated SB. The key-point is the tendency of A_{nn} to stabilize as the SB number exceeds the value 4. Besides, such effect is called the SB screening effect. Optical and SEM observations show clearly that the number of slip bands in one grain is usually much larger. It could be noticed that the stress singularity prefactor is divided by about 2 but the stress singularity exponent is still the same, α = 0.27.

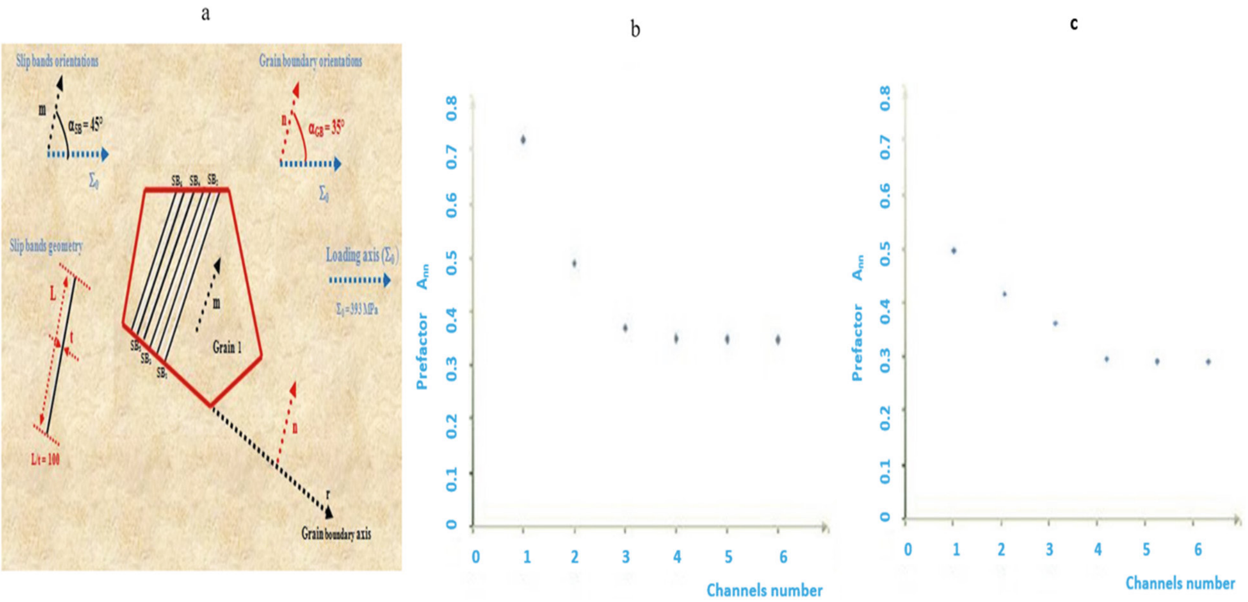

Fig. 3: a) Microstructure used in calculations b) The evolution of A_{nn} with respect of the SBs number (constant aspect ratio L/t) c) The evolution of Ann with respect of the SBs number (aspect ratio L/t varying)

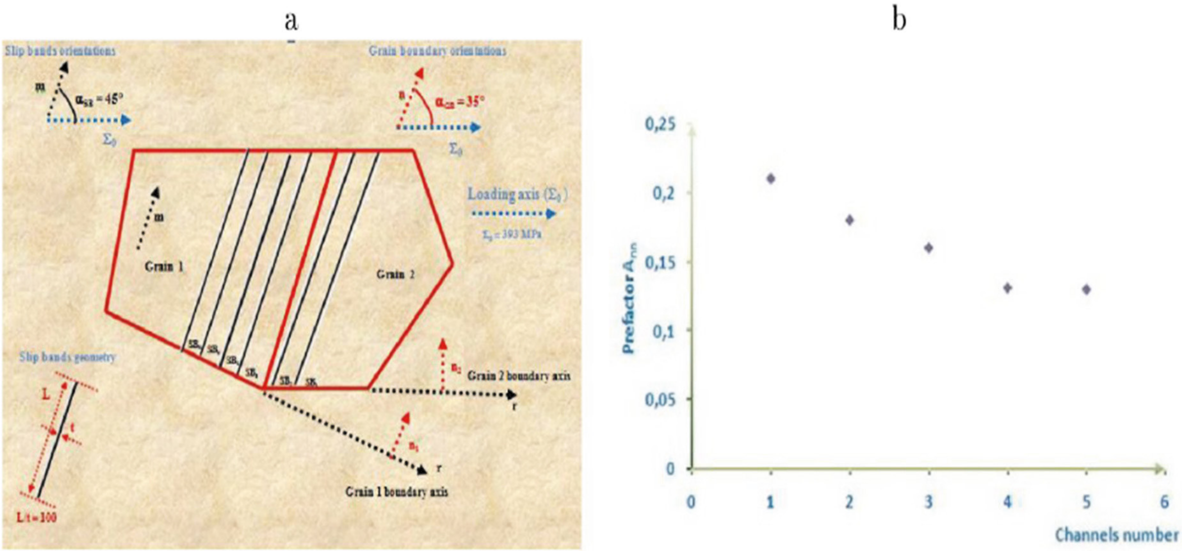

Fig. 4. a) Microstructure used in calculations b) The evolution of A_{nn} with respect of the SBs number in the case of SBs dispersed along two differently oriented GBs.

- The second configuration is the same as the first one but by changing the aspect ratio $\frac{L}{t}$, taking into account the small length variations. The loading conditions are the same as before except that the aspect ratio is slightly changed from one SB to another. According to equation (1), such aspect ratio strongly influences the GB normal stress field. One can observe (Fig. 3c) the generated drop of A_{nn} which can be explained by the screening effect.
- SBs impinge two different oriented GBs (α_{GB} = 35° and α_{GB} = 90°), see Fig. 4a. The loading conditions are the same as before except that the GBs orientations are α_{GB} = 35° and α_{GB} = 90°. One can observe that A_{nn} dramatically decreases with respect to the SBs number, beginning from SB_1 to SB_6(see Fig.4b). That is due to the combined effects of GB orientation change and screening.
- There are SBs into the two neighbor grains (Fig. 5a). Indeed, the two neighbor grains, G_1 and G_2, are plastified and slip bands impinge the GB from the two grains. But they do not connect together (no direct transmission). The loading conditions are the same as before. According to Fig 5b, in both grains, one can observe a reduction in the prefactor A_{nn} with respect to the SB number (beginning from SB1 in grain 1): such a decrease compared to the reference value is thought to be due to the screening phenomenon. Then, SBs in both the grain 1 and the grain 2 influences each other. The stress field prefactor is now divided by a factor four with respect to A_{nn}=0.27.

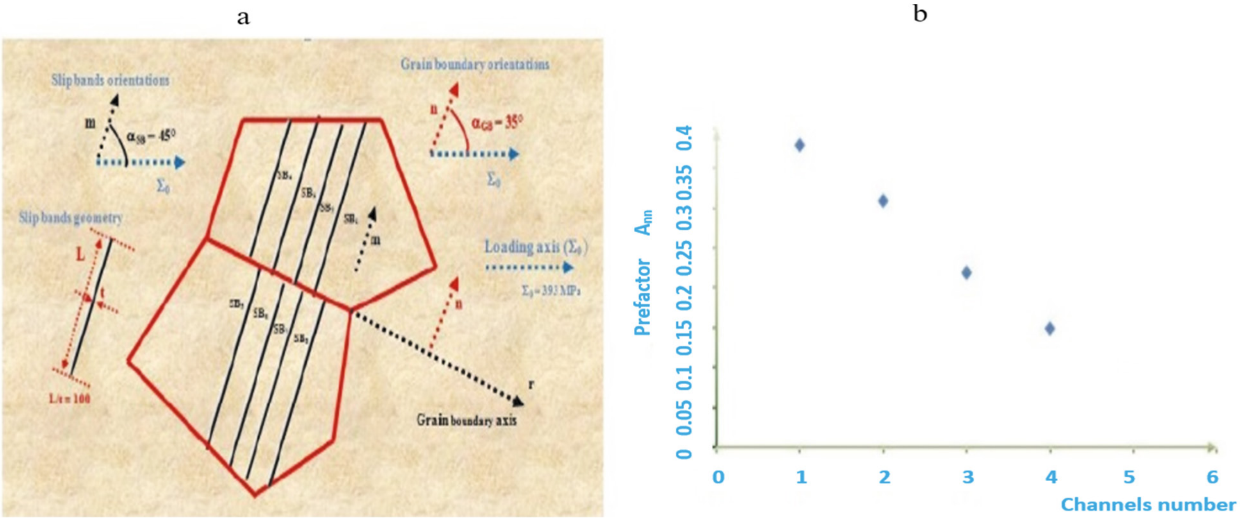

Fig. 5.a) Microstructure used in calculations b) The evolution of Ann with respect of the SBs number in the case of SBs within two neighboring grains and impinging the common GBs.

If direct transmission of plastic strain is assumed at the grain boundary. This is taken into account in building the mesh of the slip bands network by connecting them one by one, from one grain to the other one. Then the FE computations clearly show that much lower GB stresses are obtained. The GB stress singularity fields vanish as connecting the slip bands together in contrary to the case where no direct transmission is assumed (Fig. 5b). This shows clearly that direct slip transmission leads to a large GB stress decrease and consequently a much lower GB fracture sensitivity. This numerical result agrees well with the observations carried out recently by [Cui et al, 2014]. Direct transmission is indeed often observed at twin boundaries which are known to be much less prone to GB fracture.

- There is only one SB which distance from the free surface varies as shown in Fig. 6a. The loading conditions are the same as before. The distance from the free surface $\delta \in \{0.74, 1.11, 1.48, 2.23, 4.46, 6.69, 8.92\}$ μm. Fig.6b shows that the higher the distance from the free surface, δ, the lower the prefactor, A_{nn}.

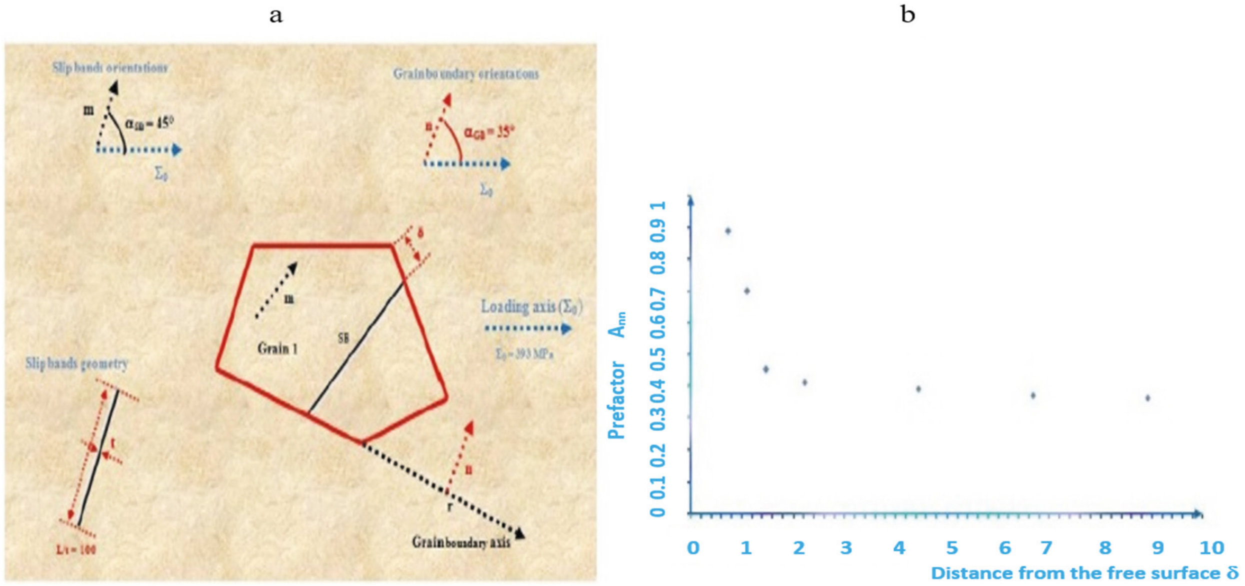

Figure 6: a) Microstructure used in calculations b) The evolution of A_{nn} with respect of the SBs number in the case of one SBs impinging the GBs at different distance from the free surface.

4. Conclusion

Taking into account slip bands of finite thickness leads to GB stress fields which are weaker than the classical pile-up ones. The deduced remote stress leading to GB fracture is closer to the measured values than the ones deduced from the pile-up theory whatever the considered environment. Usually, many slip bands are observed in each plastified grain and plastic localization may spread in the neighbor grains during straining depending on GB structure, neighbor grain orientations and tensile direction. Therefore, modeling the interactions between parallel slip bands belonging to the same grains or of slip bands belonging to two neighbor grains was required for better predicting GB stress fields and finally fracture. The screening effect of parallel slip bands leads to a decrease of a factor four in case of direct transmission. Our results agree well with many literature observations showing clearly that GB stress concentrations and the sensitivity to GB cracking is the highest as slip localization occurs in isolated grains. Then GB stress concentrations are lower and GB fracture occurs later at GBs to which slip bands impinge from the two neighbor grains. Finally, in case of direct transmission, even lower GB stresses have been measured and fracture occurs scarcely.

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