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## Influence of plastic slip localization on grain boundary stress fields and microcrack nucleation



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#### ABSTRACT

Slip localization is widely observed in metallic polycrystals after tensile deformation, cyclic deformation (persistent slip bands) or pre-irradiation followed by tensile deformation (channels). Such strong deformation localized in thin slip bands induces local stress concentrations in the quasi-elastic matrix around, at the intersections between slip bands and grain boundaries where microcracks are often observed.

Since the work of Stroh, such stress fields have been modeled using the dislocation pileup theory which leads to stress singularities similar to the LEFM ones. The Griffith criterion has then been widely applied, leading usually to strong underestimations of the macroscopic stress for microcrack nucleation.

In fact, slip band thickness is finite: 50–1000 nm depending on material, temperature and loading conditions. Then, many slip planes are plastically activated through the thickness. Stress fields have probably been overestimated using the pile-up theory which assumes that all dislocations are located on the same atomic plane. To evaluate more realistic stress fields, crystalline finite element (FE) computations are carried out using microstructure inputs (slip band aspect ratio and spacing). Slip bands (low critical resolved shear stress) are embedded in an elastic matrix. The following results are obtained concerning grain boundary normal stress fields:

- strong influence of slip band thickness close to the slip band corner, which is not
  accounted for by the pile-up theory. But far away, the thickness has a negligible effect
  and the predicted stress fields are close to the one predicted by the pile-up theory,
- analytical formulae are deduced from the numerous FE computation results which allows the prediction of surface/bulk slips as well as grain boundary stress fields. Slip band plasticity parameters, slip band length and thickness, Schmid factor and remote stress are taken into account. The dependence with respect to the various parameters can be understood in the framework of matching expansions usually applied to cracks with V notches of finite thickness,
- as the exponent of the GB stress close-field is lower than the pile-up or crack one, that is
   0.5, the Griffith criterion may not be used for GB microcrack prediction in case of finite thickness. That is why finite crack fracture mechanics is used together with both energy and stress criteria,
- the pile-up theory leads to large underestimation of the critical remote stress leading to GB microcrack nucleation measured in the case of pre-irradiated austenitic stainless steels subjected to tensile loading in inert environment, probably because of the overestimation of the local GB stress field. And the critical remote stress computed using the proposed modeling of slip bands of finite thickness is much closer to the experimental values.

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Nomenclature
           slip band thickness
t
L
           slip band length (usually one-half grain size) (or crack length when the theory of matching expansions applied to
           notches is discussed)
L<sup>pile-up</sup>
           pile-up length (usually one-half grain size)
Υ
           Young's modulus
           Poisson ratio
1)
           elastic shear modulus
μ
           length of the Burgers vector
h
d_0
           distance between two neighbour close-packed atomic planes
\Sigma_0
           remote tensile stress
           angle between the vector perpendicular to the grain boundary and the tensile direction
\sum_{n=1}^{\infty}
    =\cos^2(\alpha)\Sigma_0 remote grain boundary normal stress
           Schmid factor
G
           elastic energy release rate
           Rice integral
           grain boundary fracture energy (\gamma_{\text{fract}} = 2\gamma_{\text{s}} - \gamma_{\text{GB}})
\gamma_{\text{fract}}
           surface energy
\gamma_s
           grain boundary energy
\gamma_{GB}
           grain boundary brittle fracture stress (depending on \gamma_{\text{fract}})
\sigma_c
n_i
           unit vector perpendicular to the plane of the ith slip system (i = 1, ..., 12)
m_i
           unit slip vector of the ith slip system
|\tau_i| = |m_i^T \boldsymbol{\sigma} n_i| resolved shear stress on the ith slip system (i = 1,..., 12)
           local stress tensor (computed by the FE method)
σ
           critical shear stress on the ith slip system
\tau_{c,i}
\gamma_i^p
           plastic slip on the ith slip system
           initial critical shear stress (slip band)
\tau_0
           linear hardening slope (slip band)
H_0
           latent hardening coefficient (slip band)
а
d
           interaction matrix between the twelve FCC slip systems.
(n,m)
           activated slip system (single slip, q \gg 1)
           corresponding plastic slip (single slip, q \gg 1)
\sigma_n^{\text{pile-up}}(r,\theta) = f(r)h(\theta) GB normal stress depending on the polar coordinates, (r,\theta) (pile-up theory)
           distance to the slip band corner, measured along the GB
\theta = \alpha + 45^{\circ} angle between slip plane and grain boundary (pile-up theory)
           grain boundary normal stress field for slip bands of finite thickness, t > 0 (mainly the geometry for which \alpha = 35^{\circ}
           has been studied) T = f\Sigma_0 - (\tau_0 - H_0\gamma^p) driving shear stress
C_{surf} \approx 1.9 surface effect coefficient (type B surface slip bands)
h(\theta) = \sin \theta \cos \frac{\theta}{2} function used in the pile-up theory for expression the stress field
g(\alpha) = h(\alpha + 45^{\circ}) function used instead of h(\theta)
           geometry factor used in the formula describing stress field obtained by the theory of matching expansion
A'
           geometry factor used in the formula describing GB normal stress field computed by the FE method in case of slip
Α
           band of finite thickness, t > 0
\Sigma_c
           critical remote tensile stress leading to grain boundary microcrack nucleation (slip bands of finite thickness,
           t > 0
\Sigma_{c}^{	ext{pile-up}}
           critical remote tensile stress leading to grain boundary microcrack nucleation (pile-up theory)
\Sigma_y
           macroscopic yield stress
В
           coefficient depending on both geometry and elasticity coefficients (expression of J)
С
           coefficient depending on geometry (expression of J)
           length of crack increment
а
           length of critical crack increment
F(\theta) = (1/4)(5 + 2\cos(\theta) - 3\cos^2(\theta)) function used in the formula giving \Sigma_c^{\text{pile-up}}
\Sigma
           inverse of the ratio between the number of coincident atoms between two neighbour crystals
Σ3
           value corresponding to \Sigma = 3, that is one-third of coincident atoms. Twin boundaries display such values.
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#### 1. Introduction

Slip localization occurring at the grain scale has been extensively observed, particularly in Faced-Centred Cubic (FCC) metals and alloys subjected to either post-irradiation tensile tests [1–6] (proton or neutron irradiation with high dose), cyclic

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