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A Simplified Model for Estimating Intergranular Normal Stresses

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ABSTRACT

Intergranular stress-corrosion cracking is one of the most important ageing degradation mechanisms in polycrystalline metals. Its initiation depends on the local stress state — a microcrack along the grain boundary supposedly forms when the stress induced at its site gets above the critical value. A statistical correlation between a grain boundary type and the distribution of intergranular normal stresses on it has been identified. As it turns out, a single aptly designed parameter (effective stiffness), along with elastic anisotropy index, is sufficient for characterizing intergranular normal stress fluctuations in materials with elastic cubic grains. Its use demonstrates that the largest intergranular normal stresses most likely appear on grain boundaries whose normals are oriented along the stiffest direction in both adjacent grains. A simple bicrystal model is proposed which confirms and complements the results of numerical finite element analysis.

1 INTRODUCTION

The ability to predict most significant ageing mechanisms and material degradation modes in metallic alloys (such as austenitic stainless steels and nickel-based alloys) is of vital importance due to their widespread use in various industries, including the reactor technology (e.g. for reactor internals, pressure vessels, primary coolant circuits, ...). These processes can irreparably compromise the structural integrity of metallic components and thus shorten their service time. Particularly critical in this respect is the *intergranular stress-corrosion cracking* (IGSCC), that can affect polycrystalline aggregates under external loading when these are exposed to corrosive environment.[1] It causes the development of cracks along the *grain boundaries* (GBs).

The mechanistic (loading) aspect of IGSCC, responsible for intergranular crack formation, can to some extent be decoupled from the effect of corrosive environment and/or neutron irradiation. Those affect the physical properties and chemistry of contact surfaces and thus facilitate the growth and propagation of cracks. In the following we focus on *IGSCC initiation*, which is modelled as depending predominantly on the *intergranular normal stresses* (INS) and on the *strength* of the corresponding GBs. For a particular metallic aggregate, the intergranular

[1] In the presence of radiation, e.g. inside nuclear reactors, the conditions are even harsher since the materials are at the same time subjected to high neutron fluxes. In such case the main degradation mode is the *irradiation assisted stress-corrosion cracking* (IASCC) that causes damage even to the materials which otherwise have low susceptibility to corrosion and stress-corrosion cracking. But since irradiation does not change their elastic properties, the analysis of intergranular stresses, presented in this study, is equally applicable also for IASCC.

stresses can be accurately estimated by explicit numerical simulations. However, such an approach is computationally very demanding and highly impractical. It also provides little insight into the general features of microcrack initiation. The goal is thus to broaden our understanding of the stress-damage processes in structural materials by identifying the crucial parameters related to IGSCC initiation and constructing a simplified (semi-)analytical model, which would enable us to predict INS as a function of applied stress, material properties and type of GB.

2 GRAIN BOUNDARY TYPES

Polycrystalline materials are composed of grains. To simplify the analysis, the behaviour of IGSCC initiation is not considered here at the microstructural level. Grains are therefore treated as homogeneous and ideally elastic. This means we can neglect the presence of potential metallurgical impurities, plastic slip localizations forming dislocation channels or any other microstructural objects interacting with possible defects, even though it is known that in practice they have large effect on the local stress state at GBs and thus on intergranular crack initiation.

Grains are separated by GBs, which can be classified into different types associated with different IGSCC sensitivities. In principle each GB is unique since it is determined by slightly different values of parameters defining the exact configuration of all the grains surrounding it, accounting for their sizes, shapes, crystallographic orientations, possible defects, etc. However, by far the most relevant is the immediate neighbourhood of a GB, i.e. to a good approximation we can consider only the two grains closest (adjacent) to it and ignore the rest. On a macroscopic (*continuum*) level at which atomistic-scale degrees of freedom (d.o.f.) corresponding to arrangement of atoms on both sides of GB plane are neglected, we thus need only 5 macroscopic parameters to define a GB. One example of such set of parameters consists of the orientation of the GB plane (specified by its normal) with respect to the crystal lattices of the two grains on either side of it and the twist angle (about the GB normal) between both crystal lattices. Two grains of cubic lattice symmetry (with different crystallographic orientations) and a GB between them are depicted schematically in Fig. 1.

In principle another 2 (for uniaxial loading) or 3 (in most general case of loading) d.o.f. are needed to specify the orientation of GB normal relative to the direction of applied external loading. However, when a statistical analysis of GB stresses is performed on a large enough aggregate, such that any given GB type contains sufficiently many randomly oriented GBs that their normals cover all possible directions and are distributed uniformly on a sphere, then these additional parameters get integrated out, since there is no preferred inclination, and the 5 parameters are indeed sufficient to define a GB type. In fact even 4 are enough, since it turns out that the exact value of the twist angle is utterly unimportant for INS distributions.

3 INS DISTRIBUTIONS

Grain boundaries that belong to the same *GB type* should all have the same *GB strength*.[2] However, due to their different orientations, the corresponding stresses on them are not equal. For any given GB type a distinct *INS distribution* thus exists. In principle the wider this distribution the larger the fraction of highly stressed GBs at the same applied load and consequently the more likely the cracks are to initiate. The *stress-based criterion for microcrack formation*

[2]There are exceptions to this, related especially to the hereby-ignored atomistic degrees of freedom. One such example are the coherent Coincidence Site Lattice GBs, whose greater GB strength derives from crystal lattices on either side of GB plane sharing some lattice sites at the GB.

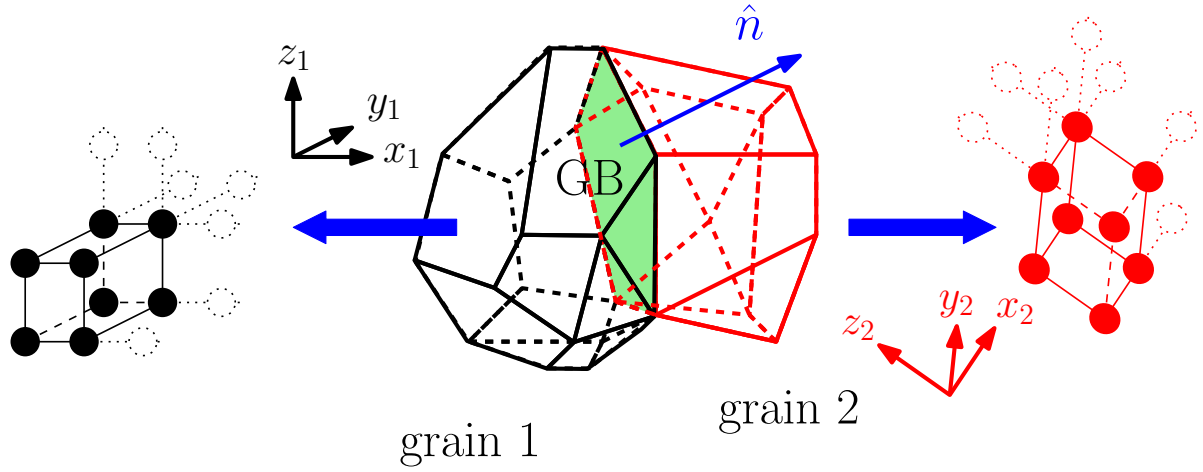

Figure 1: Grain 1 (black) and grain 2 (red) separated by a common GB (green), whose orientation is specified by its normal vector $\hat{\mathbf{n}}$. The crystallographic orientations of both grains are indicated by main symmetry axes (x_i, y_i, z_i) of the corresponding cubic lattices shown on either side.

implies that a microcrack is initiated in materials sensitive to IGSCC, whenever a local intergranular normal stress σ_{nn} is above the threshold value (determined by GB strength), i.e. for $\sigma_{nn} > \sigma_c$. The *critical stress* σ_c is assumed to depend on grain boundary type, material properties and environmental conditions, but not on a local stress, i.e. $\sigma_c \neq \sigma_c(\sigma_{nn})$. This is known as the *grain boundary stress-strength decoupling hypothesis*. It enables us to separate the treatment of local stresses σ_{nn} from the effect of exact external conditions encoded in σ_c. But note, that this is only an assumption which still requires some additional experimental verification.

Once enough microcracks form in some region (i.e. when on a sufficiently large fraction of GBs, e.g. 10%, the critical stress is exceeded), they can merge (coalesce) into a visible macroscopic crack that grows and propagates along the GBs. This can eventually lead even to failure of the entire mechanical component. Since GBs are randomly distributed (both GB normal and crystallographic orientation can be thought of as randomly assigned to each grain), the process is stochastic. The local cracking criterion introduced above can thus only be used to estimate a statistical probability for finding a macrocrack somewhere on a component's free surface, where the material is in contact with the corrosive environment. Even so, this produces a prediction, which can then be directly compared to experimental measurements (by means of High Resolution Electron Back Scatter Diffraction or Laue micro-diffraction), with the value of σ_c determined from the fitting procedure.

INS distributions can be characterized by their first two statistical moments, the *mean value* $\langle\sigma_{nn}\rangle$ and *standard deviation* $s(\sigma_{nn}) = \sqrt{\langle\sigma_{nn}^2\rangle - \langle\sigma_{nn}\rangle^2}$. Although such characterization is not unique — for that we would need to know also the higher statistical moments — it can still produce some meaningful results.

There are several relevant sources that contribute to the width of INS distribution evaluated on a particular GB type:

1. The main source is obviously the *random orientation* of GB planes. Its effect can be easily understood if one considers the *isotropic* case, for which the crystallographic orientations of grains are irrelevant and thus there is effectively only a single GB type. The direc-

tion of external macroscopic tensile loading (for simplicity taken here as uniaxial stress $\Sigma_{ZZ} := \Sigma_0$) sets a preferred direction and thus GB normal stress is $\sigma_{nn}/\Sigma_0 = \cos^2\theta$, where θ denotes the angle between a GB normal and the applied uniaxial loading direction. The INS are thus bounded by $0 \leq \sigma_{nn} \leq \Sigma_0$, with the resulting *probability density function* (PDF) of the form $dP/d(\sigma_{nn}/\Sigma_0) = 1/(2\sqrt{\sigma_{nn}/\Sigma_0})$. Its mean value and standard deviation are $\langle\sigma_{nn}/\Sigma_0\rangle = 1/3$ and $s(\sigma_{nn}/\Sigma_0) = 2/(3\sqrt{5}) \approx 0.298$, respectively.

2. If we allow for the *anisotropic* grains, but still consider all the GBs in the aggregate (despite their potentially different strengths), the INS distribution broadens, with the largest σ_{nn} exceeding the upper bound Σ_0, while on the other end it goes into negative values for the assumed tensile loading. However, irrespective of anisotropy of the grains, the largest INS is still expected on GBs with GB normals closely aligned with the applied uniaxial loading direction ($\theta \approx 0$). Standard deviation $s(\sigma_{nn}/\Sigma_0)$, measuring the width of the distribution, grows with increasing elastic anisotropy.

3. Instead on random GBs, which can have very different GB strengths, we now focus on GBs of the same type. Typically the INS distributions then adopt a bimodal shape that becomes more pronounced for stiffer GBs. The assumption is that a statistical correlation exists between a specific GB type and the corresponding INS distribution σ_{nn} on it.

Various "contributions" listed above are presented graphically in Fig. 2.

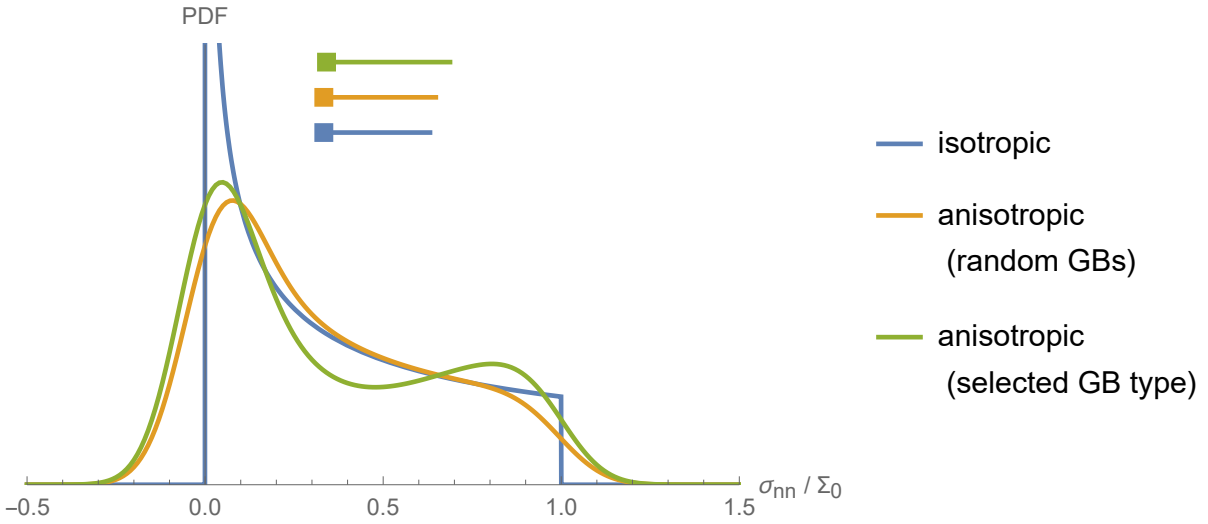

Figure 2: Illustrating the effects of GB orientation, material anisotropy and selected GB type on the shape of INS distribution represented by PDF(σ_{nn}/Σ_0). The square symbols at the top represent the mean values $\langle\sigma_{nn}/\Sigma_0\rangle$ of corresponding INS distributions while the lengths of horizontal lines to their right indicate their "widths" $s(\sigma_{nn}/\Sigma_0)$. While the latter tend to increase when we deviate from the isotropic case, the mean values always stay close to $1/3$.

4 RESULTS OF THE FINITE ELEMENT ANALYSIS

Numerical *finite element* (FE) simulations[3] demonstrate that the statistical behaviour of GB normal stresses in materials with elastic cubic grains can be accurately described for any

[3]Finite element solver Abaqus in the small strain regime was used. The applied periodic boundary conditions along all three principal directions of the aggregate imply that all the grains belong to the bulk. Since there are no free surfaces, no surface effects are involved.

GB type and loading condition by just two parameters [1]. The *Zener index* for a cubic crystal

$$A = \frac{2(s_{11} - s_{12})}{s_{44}} \tag{1}$$

is expressed in terms of its *compliance* tensor components (in Voigt notation) and characterizes the material *elastic anisotropy* (with reference value $A = 1$ denoting an isotropic crystal). The other parameter is the *effective stiffness* of the two grains along the GB normal direction,

$$E_{12} = \frac{2\overline{E}^{-1}}{E_{abc}^{-1} + E_{def}^{-1}} \,, \tag{2}$$

with $\overline{E}$ being the Young's modulus of a macroscopic untextured elastic aggregate and E_{abc} and E_{def} denoting the Young's moduli of both grains along their respective GB normal directions (a, b, c) and (d, e, f),

$$E_{abc}^{-1} = s_{11} - 2s_0 \frac{(ab)^2 + (ac)^2 + (bc)^2}{(a^2 + b^2 + c^2)^2} \,, \tag{3}$$

for $s_0 := s_{11} - s_{12} - \frac{s_{44}}{2} = \frac{s_{44}}{2}(A-1)$. The newly introduced E_{12} parameter measures the average stiffness of GB's immediate neighbourhood along the GB normal direction. The amplitude of INS fluctuations, measured by $s(\sigma_{nn}/\Sigma_0)$, reduces if both grains are softer than the surrounding material and thus the applied stress, projected along the GB normal, redistributes more over the stiffer bulk than over the softer grains. Conversely, the largest normal stresses most likely form on GBs whose normals are oriented along the stiffest direction in both adjacent grains. This allows for a simple classification of GBs according to their tendency for adopting large stresses and leads to certain interesting implications for Coincidence Site Lattice GBs. For instance, the coherent Σ_3-twin GB, known experimentally for its high cracking resistance [2], was shown to experience disproportionately large INS. This indicates its exceptionally large GB strength [3].

The amplitude of INS fluctuations seems very well-correlated with the value of E_{12}. Points obtained in FE simulations can be fitted by

$$s(\sigma_{nn}/\Sigma_0) = A_1 \arctan\left(A_2 E_{12}^{A_3}\right) \,, \tag{4}$$

and the agreement is very good [1]. Fitting coefficients A_k are material-specific, but seem to depend only on elastic anisotropy A, possibly also on the loading type. The effect of increased anisotropy is clearly visible in Fig. 3.

The *effective GB stiffness* E_{12} combines the geometrical aspect of each GB type (related to the 4 parameters mentioned earlier – the unit length vectors (a, b, c) and (d, e, f)) with its material properties (the values of s_{ij}) in such a way that different GB types (with in principle different GB strengths) are grouped together when their INS distributions have the same width. Consequently, when going over all the GB types (or even over all the GBs) in the aggregate and assigning appropriate E_{12} values to them (which are directly related to their INS fluctuation amplitudes), it turns out that not all values of E_{12} appear equally often. The reason is that to some values of E_{12} more GB types correspond to and to some less. For instance, while (a, b, c) directions $(1, 0, 1)$, $(1, 1, 2)$ and $(3, 1, 4)$ are completely different (i.e. are not related by any symmetry) and thus denote different GB types, they still lead to the same value of E_{abc} and thus the same E_{12}. On the other hand the softest and the stiffest crystal directions corresponding to minimal and maximal value of E_{12}, respectively, do not show this kind of "degeneracy". This can be observed for several chosen materials in Fig. 4 and is important for understanding the

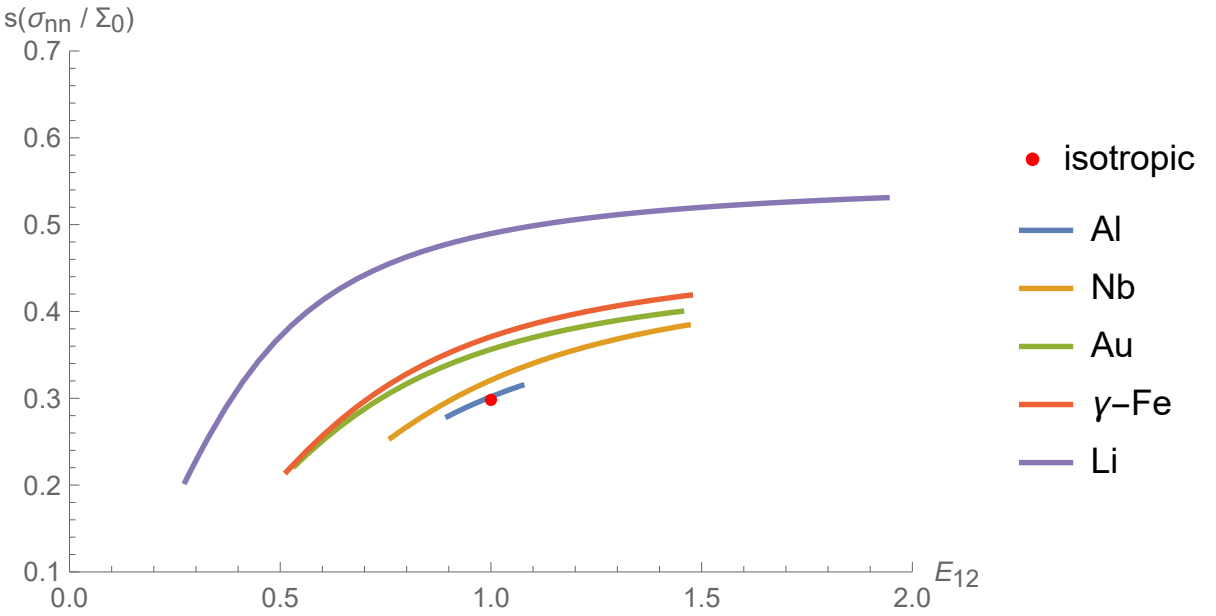

Figure 3: Standard deviation $s(\sigma_{nn}/\Sigma_0)$ as a function of GB stiffness E_{12}, cf. Eq. (4). Different materials are presented with different values of Zener index A determining the fitting coefficients A_k. For comparison also isotropic case ($A = 1$) is shown.

INS distribution on random GBs (represented for instance by the yellow curve in Fig. 2) — obviously some values of E_{12} will contribute a lot more to it than others.

Even though the phenomenological relation between the INS fluctuation amplitude and the corresponding GB type in Eq. (4) has been derived assuming *uniaxial tensile loading*, similar relations can be formulated even for other types of loading (such as a *general triaxial loading*), with the characteristic parameter E_{12} still playing a pivotal role.

5 SIMPLIFIED BICRYSTAL MODEL

To provide a more intuitive explanation of our findings, a simplified *bicrystal model* embedded in an isotropic elastic medium will be used. With it the significance of effective GB stiffness E_{12} can be further substantiated.

To assess analytically the normal stress at a GB between a pair of grains composing a bicrystal, we need to solve a system of constitutive equations — the generalized Hooke's law:

$$\epsilon_{ij} = s'_{ijkl}\sigma_{kl} \,, \quad i,j,k,l = 1,2,3 \,, \tag{5}$$

where ϵ_{ij}, s'_{ijkl} and σ_{kl} are the components of strain, compliance and stress tensors, respectively. Summation over repeated indices is implicit. Strain tensor is symmetric ($\epsilon_{ij} = \epsilon_{ji}$) and similarly stress tensor ($\sigma_{ij} = \sigma_{ji}$). In a local coordinate system aligned with crystallographic axes of a grain with cubic symmetry, the only non-vanishing components of compliance tensor s_{mnop} are

$$s_{mmmm} \equiv s_{11} \,, \quad m = 1,2,3 \,, \tag{6}$$

$$s_{mnmn} = s_{mnnm} \equiv \tfrac{1}{4}s_{44} \,, \quad m,n \neq m = 1,2,3 \,, \tag{7}$$

$$s_{mmnn} \equiv s_{12} \,, \quad m,n \neq m = 1,2,3 \,, \tag{8}$$

depending on just 3 parameters. Since we are interested in a GB normal stress, it is easiest to express all the quantities in a GB system (that has z-axis oriented along the GB normal) and

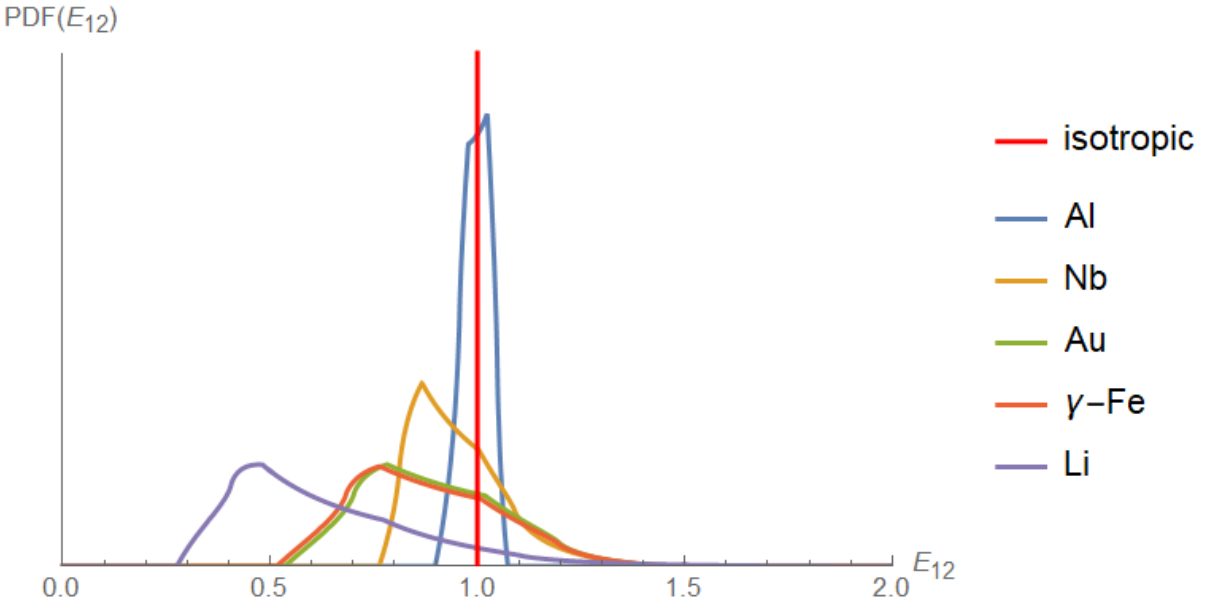

Figure 4: Probability density function (PDF) with respect to the value of GB stiffness E_{12}, defined in Eq. (2), for a few selected materials arranged in increasing order of anisotropy (specified as departure from the isotropic case $A = 1$). The corresponding Zener indices are: $A(\text{Al}) = 1.22$, $A(\text{Nb}) = 0.49$, $A(\text{Au}) = 2.85$, $A(\gamma\text{-Fe}) = 3.37$ and $A(\text{Li}) = 8.52$.

compute σ_{zz}. To transform the compliance tensor to a GB system, it needs to be rotated by an orthogonal rotation matrix $\mathbf{R}$ representing a general (passive) rotation from the crystallographic coordinate system $(\mathcal{X}, \mathcal{Y}, \mathcal{Z})$ of a grain to a (x, y, z) system of a GB:

$$\begin{aligned} s'_{ijkl} &= \sum_{m,n,o,p=1}^{3} R_{im} R_{jn} R_{ko} R_{lp}\, s_{mnop} \\ &= \sum_{m=1}^{3} (R_{im} R_{jm} R_{km} R_{lm}) \cdot s_0 + \delta_{ij}\delta_{kl} \cdot s_{12} + (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \cdot \frac{s_{44}}{4}\,, \end{aligned} \tag{9}$$

where $\mathbf{R}$ is in general a function of 3 Euler angles. Eq. (5) needs to be solved for each of the two grains — the 24 variables (6 stress and 6 strain components in each grain) are connected by 12 coupled equations and the same number of *boundary conditions* corresponding to:

1. *stress continuity across the GB*

$$\sigma^{(1)}_{xz} = \sigma^{(2)}_{xz} \quad , \quad \sigma^{(1)}_{yz} = \sigma^{(2)}_{yz} \quad , \quad \sigma^{(1)}_{zz} = \sigma^{(2)}_{zz}\,, \tag{10}$$

2. *strain compatibility across the GB*

$$\epsilon^{(1)}_{xx} = \epsilon^{(2)}_{xx} \quad , \quad \epsilon^{(1)}_{xy} = \epsilon^{(2)}_{xy} \quad , \quad \epsilon^{(1)}_{yy} = \epsilon^{(2)}_{yy}\,, \tag{11}$$

3. *average strain of the bicrystal*

$$\begin{aligned} V_1\,\epsilon^{(1)}_{xx} + V_2\,\epsilon^{(2)}_{xx} &= (V_1+V_2)\,\bar{\epsilon}^{b}_{xx} \quad , \quad V_1\,\epsilon^{(1)}_{yz} + V_2\,\epsilon^{(2)}_{yz} = (V_1+V_2)\,\bar{\epsilon}^{b}_{yz}\,, \\ V_1\,\epsilon^{(1)}_{yy} + V_2\,\epsilon^{(2)}_{yy} &= (V_1+V_2)\,\bar{\epsilon}^{b}_{yy} \quad , \quad V_1\,\epsilon^{(1)}_{xz} + V_2\,\epsilon^{(2)}_{xz} = (V_1+V_2)\,\bar{\epsilon}^{b}_{xz}\,, \\ V_1\,\epsilon^{(1)}_{zz} + V_2\,\epsilon^{(2)}_{zz} &= (V_1+V_2)\,\bar{\epsilon}^{b}_{zz} \quad , \quad V_1\,\epsilon^{(1)}_{xy} + V_2\,\epsilon^{(2)}_{xy} = (V_1+V_2)\,\bar{\epsilon}^{b}_{xy}\,, \end{aligned} \tag{12}$$

with V_1 and V_2 denoting the volumes of respective grains. The strain ϵ_{ij} is assumed constant throughout each grain (mechanical equilibrium) and $\bar{\epsilon}^b_{ij}$ is the average strain of a bicrystal.

With that we can in principle solve the equations for any pair of grains in the aggregate if we only know the value of $\bar{\epsilon}^b_{ij}$. The problem is that the latter depends not only on external loading Σ^{ext}_{ij} (expressed in a GB system) but also on the specifics of a selected bicrystal pair and its position within the aggregate. That means we need to know the exact configuration of all the grains in it to solve the system. Sensible approximation would thus be to treat the neighbourhood of an investigated pair of grains as a homogeneous and isotropic matrix material with average bulk properties. By matching $\bar{\epsilon}^b_{ij}$ to the macroscopic strain $\bar{\epsilon}_{ij}$ of the polycrystalline aggregate, we can then relate it to the average Young's modulus $\overline{E}$ and Poisson's ratio $\bar{\nu}$ of the specimen, where both of these are only functions of material properties s_{11}, s_{12} and s_{44}:

$$\bar{\epsilon}^b_{ij} = \bar{\epsilon}_{ij} = \frac{1+\bar{\nu}}{\overline{E}}\Sigma^{ext}_{ij} - \frac{\bar{\nu}}{\overline{E}}(\mathrm{Tr}\,\boldsymbol{\Sigma}^{ext})\,\delta_{ij}\ , \tag{13}$$

$$\overline{E} = \frac{9KG}{3K+G}\ , \tag{14}$$

$$\bar{\nu} = \frac{3K-2G}{2(3K+G)}\ , \tag{15}$$

with compression and shear elastic moduli defined as

$$K = \frac{1}{3(s_{11}+2s_{12})}\ , \tag{16}$$

$$G = \begin{cases} 8(s_{11}+2s_{12})(s_{11}-s_{12})s_{44}\,G^3 + (5s_{11}+s_{12})s_{44}\,G^2 - (7s_{11}+11s_{12})\,G = 1 \\ G > 0 \end{cases}\ . \tag{17}$$

Even with this simplification the system is still too complicated to be solved analytically, but at least the equations can be dealt with numerically (for any chosen material and type of loading). Let us first consider a case of macroscopic *uniaxial* tensile loading, that we can directly compare to the results of FE analysis described in the previous section. Its stress tensor written in a global (lab) coordinate system (X, Y, Z), associated with applied external loading, is

$$\boldsymbol{\Sigma}^{ext} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \Sigma_0 \end{pmatrix}. \tag{18}$$

When rotated (projected) into a local GB system (x, y, z), it takes the following form

$$\mathcal{R}\boldsymbol{\Sigma}^{ext}\mathcal{R}^T = \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} & \Sigma_{xz} \\ \Sigma_{xy} & \Sigma_{yy} & \Sigma_{yz} \\ \Sigma_{xz} & \Sigma_{yz} & \Sigma_{zz} \end{pmatrix} = \Sigma_0 \begin{pmatrix} \cos^2\phi\sin^2\theta & -\cos\phi\sin\phi\sin^2\theta & -\cos\phi\cos\theta\sin\theta \\ -\cos\phi\sin\phi\sin^2\theta & \sin^2\phi\sin^2\theta & \sin\phi\cos\theta\sin\theta \\ -\cos\phi\cos\theta\sin\theta & \sin\phi\cos\theta\sin\theta & \cos^2\theta \end{pmatrix}, \tag{19}$$

which in general depends on 2 spherical angles θ and ϕ (where ϕ can be set to any value and thus drops out — fixing of ϕ corresponds only to from-a-physics-perspective irrelevant choice of x and y axes in the GB plane). Note that for multiaxial types of loading (e.g. for a general *triaxial* tensor considered later), there is one more independent parameter (additional angle φ) needed to specify the rotation by matrix $\mathcal{R}$.

This allows us to numerically solve the system of equations (5) with boundary conditions (10)–(12) (assuming (13) and grains of equal size $V_1 = V_2$) for any chosen material and type of loading. Basically we are performing a Monte-Carlo simulation: by fixing the direction of GB normal with respect to crystal lattices of both adjacent grains (a, b, c, d, e, f) we are choosing a specific GB type. Then we randomly sample over possible orientations of the GB plane with respect to the lab system (X, Y, Z). This gives us an INS distribution for which we can compute its standard deviation $s(\sigma_{zz})$. Each such computation (corresponding to a selected GB type) represents a single point on the scatter plot in Fig. 5 that was computed for γ-Fe ($s_{11} = 9.94\,\mathrm{TPa}^{-1}$, $s_{12} = -3.85\,\mathrm{TPa}^{-1}$, $s_{44} = 8.20\,\mathrm{TPa}^{-1}$) under uniaxial tensile loading (18).

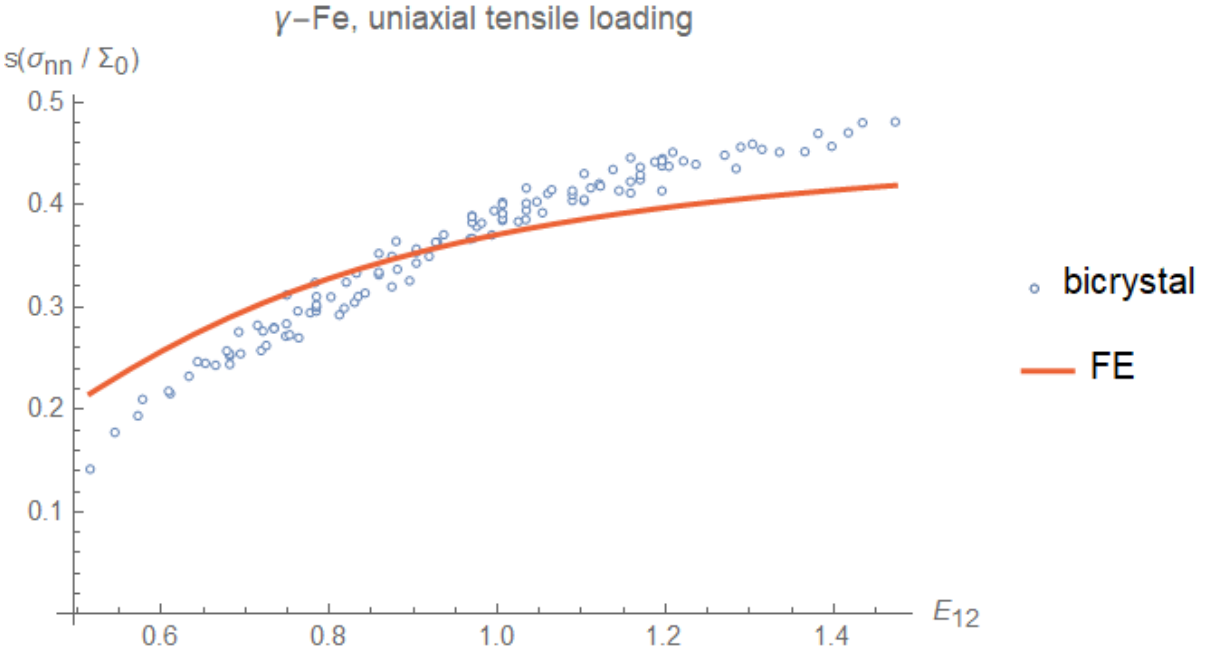

Figure 5: Standard deviation $s(\sigma_{nn}/\Sigma_0)$ as a function of GB stiffness E_{12} for γ-Fe and uniaxial loading. Comparison is made between the results of FE simulation and the solution of a simplified bicrystal model.

The results again reveal a very strong correlation between the parameter E_{12} (2) and the width of associated INS distribution. Comparison with FE results shows that both methods produce similar monotonic trends but with slightly different slopes. This discrepancy can be attributed to incorrect boundary conditions in our bicrystal model approach — if the GB is soft (i.e. corresponding to a small E_{12}), both its tensile and compressive strains should be larger than the average aggregate's value $\bar{\epsilon}_{ij}$ and thus the magnitude of stress bigger than in approximation (13). The true value of standard deviation (represented by FE result) should therefore exceed the bicrystal estimate. The opposite is true for very stiff GBs (corresponding to a large E_{12}).

We can also consider other types of loading. For instance, a most general *triaxial* stress tensor is of the form

$$\boldsymbol{\Sigma}^{ext} = \Sigma_0 \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix}. \tag{20}$$

Its components expressed in a GB system (Σ_{ij}^{ext}) are now more complicated functions of α, β, γ, φ, θ and ϕ (where the value of ϕ can again be fixed), but otherwise the procedure is very similar to the uniaxial case. Three different types of loading are compared in Fig. 6.

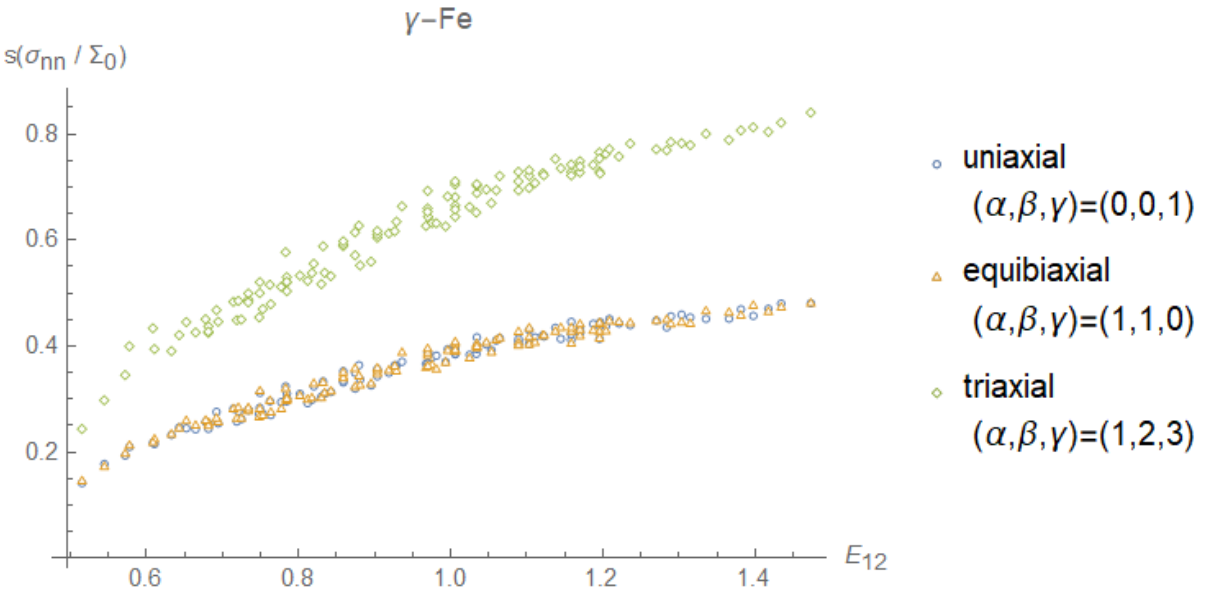

Figure 6: Standard deviation $s(\sigma_{nn}/\Sigma_0)$ as a function of GB stiffness E_{12}. All curves correspond to the solutions of a bicrystal model with γ-Fe grains but for different types of loading.

In conclusion, E_{12} from Eq. (2) remains a good quantity for specifying σ_{nn} fluctuations even for an arbitrary uniform loading.

6 CONCLUSIONS

The long-term goal is to become capable of predicting IGSCC initiation as a function of the applied external stress. This would be especially relevant for improving our understanding of the ageing degradation phenomena and potentially even design materials with improved cracking resistance in the future.

As a first step towards that we were trying to model the distribution of GB stresses on each particular GB type. It turns out that its first two statistical moments[4] depend on just two carefully chosen parameters — Zener anisotropy index and the effective GB stiffness. The main result of our numerical finite element analysis could thus be expressed in layman's terms as follows: the seemingly almost trivial realization is that "the stiffer the GB the larger the stress on it (both tensile and compressive) and thus the larger the width of the corresponding distribution", while the less trivial conclusion is that this stiffness can be quantitatively (quite precisely) characterized by the hereby introduced E_{12} parameter.

A simple bicrystal model was presented whose biggest weakness lies in our ignorance of the exact boundary conditions, which prevents us from solving the system of constitutive equations for a chosen pair of grains. We thus had to further simplify our approach by taking certain plausible approximations, which allow us to obtain the solution numerically. The agreement with finite element results is quite good and provides additional support for our main claim — the importance of E_{12} for characterizing the probability for large normal stresses to arise.

What remains to be done, is to construct an accurate analytical model of INS distributions for any GB type, type of loading and material, i.e. to go beyond their first two statistical moments approximation. The actual shape of σ_{nn}/Σ_0 distributions (and not just the corresponding standard deviations $s(\sigma_{nn}/\Sigma_0)$ of the normalized INS) is needed to measure the fraction of GBs

[4] In fact only standard deviation varies with GB type while the mean value remains almost constant.

with large normal stresses. Knowing the value of σ_{nn} (or ideally even how to express it in analytical form) on any particular GB, would allow us to quickly estimate INS distributions without having to rely on numerical simulations.

Once this is successfully achieved, the next logical step would be the following: assuming that INS-based criterion for microcrack formation applies[5], the strength of a selected GB type could be determined experimentally by simply checking what fraction of its GBs cracked under loading. Since different GB types can have the same effective stiffness E_{12} and thus the same width of INS distribution, their GB strengths can be directly compared — the type with smaller fraction of cracked GBs is the more resistant one.

ACKNOWLEDGMENTS

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[5] Assumption of a continuum limit is crucial for that since it allows us to treat the grains and GBs as featureless objects and thus GBs of the same type as having the same GB strength.