Theoretical approach to the ductile fracture of polycrystalline solids

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It is shown here that fracture after a brief plastic strain, typically of a few percents, is a necessary consequence of the polycrystalline nature of the materials. The polycrystal undergoing plastic deformation is modeled as a flowing continuum of random deformable polyhedra, representing the grains, which fill the space without leaving voids. Adjacent grains slide with a relative velocity proportional to the local shear stress resolved on the plane of the shared grain boundary, when greater than a finite threshold. The polyhedral grains reshape continuously to preserve matter continuity, being the forces causing grain sliding dominant over those reshaping the grains. It has been shown in the past that this model does not conserve volume, causing a monotonic hydrostatic pressure variation with strain. This effect introduces a novel concept in the theory of plasticity because determines that any fine grained polycrystalline material will fail after a finite plastic strain. Here the hydrostatic pressure dependence on strain is explicitly calculated and shown that has a logarithmic divergence which determines the strain to fracture. Comparison of theoretical results with strains to fracture given by mechanical tests of commercial alloys show very good agreement.

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I. INTRODUCTION

Asking why things break when subjected to strong enough forces may sound superfluous because breaking objects is one of the most early experiences of every person. In reality, explaining why solids undergoing plastic deformation are unable of achieving a steady flow regime and collapse past a finite plastic flow, or with almost no flow at all, is a most important scientific and technical problem yet unsolved. In technical grounds the point is quite serious because of the high expenses associated to fatigue and failure of functional articles. As well, the design of machine parts and structures is always restricted by the strength of the materials they will be made of, which puts limits to their efficiency and bounds costs from below. Since the early investigations of Griffith [1], who claimed that the tensile strength of glass is lowered by the presence of very small pre-existent cracks that concentrate stresses when the material is loaded, and Irwin [2] and Orowan [3], who extended the idea to ductile solids, a great amount of effort has been expended in elucidating why solid materials break from the atomic point of view.

Nowadays the question has turned to how solids fail, instead of why they break. Certainly, the two issues are closely related and answering the former question may clarify the latter, but not necessarily. Most of the contemporary research on this subject relies on the hypothesis of cracks, and ascribes brittle behavior to the ability of stressed crack tips to propagate conserving their atomically sharp edges. In ductile solids the tip of the crack blunts, broadens and flows, demanding increasing effort to make it progress [4–10]. Unfortunately, the problem of stress induced crack propagation has proven to be exceedingly complex, and neither theory nor computer simulations [11,12] have produced conclusive answers on the fracture process and the origin of brittle or ductile fracture. The complex evolution of crack growth has been accurately measured [14–16], confirming atomic scale model predictions [17,18] that the dynamics of a crack tip is highly unstable, and steady motion in a given direction is in most situations impossible.

We show here that the reason why continued deformation inevitably makes solids to break, undergoing either brittle, ductile or superplastic fracture, is much more basic and simpler than how fracture proceeds. Resorting to a very general model for the structure of the solid, we demonstrate in what follows that fine grained polycrystalline materials are not able of a steady flow, no matter the strength of the forces involved, and should collapse after reaching a finite plastic strain.

At a scale much larger than the grain size, polycrystalline matter lacks symmetry constrictions and periodicity, and displays same average packing and properties in all directions, and over its whole extent. Despite this, assimilating an even very fine grained polycrystal to an homogeneous and isotropic continuum may lead to gross errors, no matter the scale, when dealing with it as a dynamical medium. The faceted nature of the structural constituents of a polycrystal determines that the force fields governing their plastic flow yield $\nabla \cdot \vec{v} \neq 0$, $\vec{v}$, $\nabla$.
where \( \vec{v} \) is the velocity field of the material continuum. This means that flow makes the specific volume to vary. Grain elasticity in polycrystalline solids allows for some density variation, and hence the medium can flow up to some limit, yielding ductile behaviour. However, the consequent pressure build up influences strongly the ongoing deformation, which cannot be steady, and finally produces fracture. Thus ductility is closely related to compressibility.

II. THEORY

A. The force model

The model for the plastic flow of a polycrystalline solid has been extensively studied, principally in the context of superplasticity, but is expected to equally hold for normal ductile solids. However, a brief account of its physical basis and the resulting general theoretical scheme is in order here.

The plastic deformation of a fine grained polycrystalline solid is modelled as a flowing continuum of random irregular polyhedra of different shapes and sizes, representing grains, which share faces. The model is essentially the same as the one of Ref. [19]. Grains can move over long paths by sliding along the shared surfaces, or grain boundaries, accommodating effortlessly their shapes to preserve matter continuity. Certainly, grain shape accommodation demands some effort, but it is assumed much smaller than the one required for grain sliding. In other words, the shear stress between two sliding grains is greater than the critical resolved shear stress (CRSS) demanded by slip deformation of the crystallites. This way, grain boundary sliding is the rate limiting process in the plastic strain. In the present scheme grains always retain their individuality and mass, and are the dynamical entities. The flow is driven by a field of tensor forces between the grains, determined by the stress tensor.

Fig. 1 shows a local frame of reference \((x'y'z')\) with the \(x'y'\) plane coincident with the boundary between two adjacent grains. The total shear stress in the shared boundary plane then reads \(\tau_{z'} = (\sigma_{x'z'}^2 + \sigma_{y'z'}^2)\), where \(\sigma_{x'z'}, \; i', j' = x', y', z'\), stands for the components of the stress tensor in this local coordinate system. There is strong evidence that the sliding relative speed \(|\Delta \vec{v}|\) of two adjacent grains obeys a linear law of the general form \(|\Delta \vec{v}| = Q(\tau_{z'} - \tau_c)\) for \(\tau_{z'} > \tau_c\) in plastic deformation [19–24]. Here \(Q\) is a proportionality coefficient and \(\tau_c\) is a critical shear stress such that \(|\Delta \vec{v}| = 0\) when \(\tau_{z'} = \tau_c\). As \(\Delta \vec{v}\) is parallel to the shear force in the plane of the interface, its components are given by \(\Delta v_{i'} = Q(\tau_{z'} - \tau_c)(\sigma_{i'z'}/\tau_{z'}), \; i' = x', y', \; z', \; \tau_{z'} \geq \tau_c\). This expression for \(\Delta \vec{v}\) has proven to hold with great accuracy for several aluminium, titanium and magnesium alloys [24–20]. Hence the force law at the grain scale reads

\[
\Delta v_{i'} = \begin{cases} 
Q \left( 1 - \frac{\tau_c}{\tau_{z'}} \right) \sigma_{i'z'}, & i' = x', y', \text{if } \tau_{z'} > \tau_c \\
0, & \text{otherwise},
\end{cases}
\]

(1)

The coefficient \(Q = Q(p, T)\) does not depend on the shear stresses and neither on the orientation of the grain boundary, therefore its dependence on the normal stresses is only via the hydrostatic pressure invariant

\[
p = -(\sigma_{x'z'} + \sigma_{y'y'} + \sigma_{z'z'})/3.
\]

(2)

The next step is to express the force law (1) in the frame of reference \((xyz)\), common to all grain surfaces, instead of the local ones \((x'y'z')\). Given the rotation matrix \(R(\theta, \phi) = (R_{ij}(\theta, \phi))\) connecting the two frames one can put the local stress tensor

\[
(\sigma_{i'j'}) = R(\theta, \phi)(\sigma_{ij})R^T(\theta, \phi)
\]

(3)

in terms of the stress tensor \((\sigma_{ij})\) of the externally applied forces and the Euler angles \((\theta, \phi)\) of the grain boundary plane. The macroscopic force law is obtained from replacing in Eq. (1) and averaging over the Euler angles. Invoking also Hooke's law one has that

\[
\nabla \cdot \vec{v} = \frac{\dot{V}}{V} = -\frac{\dot{p}}{B},
\]

(4)

where \(B\) is the bulk elastic modulus, \(\dot{p}\) the pressure variation rate, and \(\dot{V}/V\) the volume variation rate per unit
B. The equations of motion

After a rather tedious set of mathematical steps the procedure outlined above for the special case of an externally applied unidirectional normal stress \( \sigma \) on a polycrystalline solid, isotropic in the scale much larger than the mean grain size \( d \), yields the complete set of macroscopic equations of motion

\[
\dot{\varepsilon} = s \frac{\tau_c Q(p)}{2d} \left[ \cot(2\theta_c) + 2\theta_c - \frac{\pi}{2} \right], \tag{5}
\]

\[
\dot{p} = s B \frac{\tau_c Q(p)}{2d} \left[ \frac{1 - \cos(2\theta_c)}{\sin(2\theta_c)} - 2\theta_c \left( 1 + \frac{2}{\pi \sin(2\theta_c)} \right) \right], \tag{6}
\]

where \( \dot{\varepsilon} \) is the strain rate in the direction of the applied stress \( \sigma \), \( s = \pm 1 \) assumes the positive and negative values for tension and compression, respectively, and the auxiliary variable \( \theta_c \) is given by

\[
\sin(2\theta_c) = \frac{4\tau_c}{3|\sigma + p|}. \tag{7}
\]

The properties of the specific material enter the theoretical formulation through the coefficient \( Q(p,T) \), governing grain boundary sliding. It has been studied in detail for fine grained polycrystalline solids and has been shown to be of the general form

\[
\frac{Q(p,T)}{4d} = C_0 \frac{\Omega^*}{k_BT} \exp \left( -\varepsilon_0 + \Omega^* p \right), \tag{8}
\]

where \( k_B \) is the Boltzmann constant, \( T \) the absolute temperature, the coefficient \( C_0 \) depends only on the grain size \( d \), the constant \( \varepsilon_0 \) is the energy necessary for evaporating a crystal vacancy from the grain boundary, and \( \Omega^* \) is the excitation volume for the same process.

Eqs. (5), (6) and (7) show that plastic flow is essentially a time dependent problem. They govern the coupled time evolution of the three variables, \( \sigma, \varepsilon \) and \( p \), relevant for the cylindrically symmetric deformation of a polycrystalline continuous medium. The actual behaviour of these variables in specific circumstances depends also on the initial conditions and deformation path (\( \sigma = \text{constant}, \ \dot{\varepsilon} = \text{constant} \), or any other imposed condition between the variables and their time derivatives).

The observed dependence on history of the plastic properties of ductile solids is usually attributed to structural variations or deformation induced damage. In the present scheme, history enters through the initial condition for the variable \( p \), which is omitted in the traditional theoretical approaches to plasticity. Here, the system described by Eqs. (5), (6) and (7) behaves always the same way, but its evolution depends on the initial conditions for the variables, which include \( p \). In opposition to the classical theory of plasticity, it exists a nontrivial transversal stress \( \sigma_\perp = -(\sigma + 3p)/2 \) which is not an independent variable, but evolves in time as dictated by the equations of motion. One can set \( \sigma_\perp = 0 \) as a natural initial condition if the material has been previously annealed, but \( \sigma_\perp \) is expected to take finite values on the subsequent deformation. As the magnitude inside the square brackets in the right hand side of Eq. (4) is positive for any \( \theta_c, \ \dot{p} \) has the sign of \( s \). The transversal stress \( \sigma_\perp \) then decreases monotonically to negative values for positive \( \sigma + p \). Physically, this means that the plastic stretching in one direction is always accompanied by a finite compression in the plane normal to the deformation axis, which increases monotonically with strain. This explains why necking always precedes ductile fracture.

C. The equations for constant strain rate

Replacing Eq. (6) in the identity \( d\varepsilon = (\dot{\varepsilon}/\dot{p}) dp \) one has that

\[
d\varepsilon = s \frac{2\dot{\varepsilon} d}{B\tau_c} \left[ \frac{1 - \cos(2\theta_c)}{\sin(2\theta_c)} - 2\theta_c \left( 1 + \frac{2}{\pi \sin(2\theta_c)} \right) \right]^{-1} \frac{\dot{p}}{Q(p,T)}, \tag{9}
\]

where \( \dot{\varepsilon} \) is considered as a given constant. As long as \( \dot{\varepsilon} = \text{constant} \), Eq. (10) shows that \( \theta_c = \theta_c(p) \). Combining the derivatives of Eqs. (5) and (8) with respect to \( p \) it can be shown that

\[
\frac{dp}{Q} = -s \frac{k_B T}{\Omega^* \dot{\varepsilon}} \frac{\tau_c}{d} \cot^2(2\theta_c) d\theta_c. \tag{10}
\]

Replacing now Eq. (10) in (9) and integrating, it is finally obtained

\[
\varepsilon = -\frac{2k_B T}{B\Omega^*} \int_{\theta_0}^{\theta_c} d\theta \cot^2(2\theta_c) \left[ \frac{1 - \cos(2\theta)}{\sin(2\theta)} \right]^{-1} \left[ 2\theta_c \left( 1 + \frac{2}{\pi \sin(2\theta_c)} \right) - \frac{2}{\pi} \cos(2\theta) + \frac{\pi}{2} \right], \tag{11}
\]

where the limits \( \theta_0 \) and \( \theta_c \) correspond to the critical angles for the initial and final values of the strain, \( \varepsilon = 0 \) and \( \varepsilon \), respectively. This way, \( \varepsilon \) is related with the auxiliary variable \( \theta_c \) by an expression of the form

\[
\varepsilon = \frac{k_B T}{B\Omega^*} [F(\theta_c) - F(\theta_0)] \ (\dot{\varepsilon} = \text{constant}), \tag{12}
\]
where $F(\theta)$ is the universal function

$$F(\theta) = -2 \int_{\pi/8}^{\theta} d\theta \cot^2(2\theta) \left[ \frac{1 - \cos(2\theta)}{\sin(2\theta)} \right] - 2\theta \left( 1 + \frac{2}{\pi \sin(2\theta)} \right) - \frac{2}{\pi} \cos(2\theta) + \frac{\pi}{2} \right]^{-1},$$

(13)

which is monotonically decreasing in its whole range $(0, \pi/4)$ and has two singularities, at $\theta = 0$ and $\theta = \pi/4$. If the material has been thoroughly annealed prior to the plastic deformation, it holds the initial condition $p = -\sigma_0/3$ at $\varepsilon = 0$, where $\sigma_0$ is the stress at the beginning of the plastic deformation.

The magnitude of $\varepsilon$ is controlled by the adimensional coefficient appearing in Eqs. (11) and (12), which is a very small quantity. The bulk modulus $B$ for metals is of the order of $10^{11}$ Pa. Previous literature on aluminium and titanium alloys shows that $\Omega^*$ is $2.6 \times 10^{-27} m^3$ for Al $\approx$ 8090 and $5.9 \times 10^{-28} m^3$ for titanium Ti–6Al–4V at rather high temperatures $[24]$. Assuming $\Omega^*$ does not vary too much with $T$ one can take these figures to estimate that, at $T = 300 K$,

$$\frac{k_B T}{\Omega^*} \sim 2.3 \times 10^{-5} - 7.0 \times 10^{-5}.$$  

(14)

Because of the small value of the coefficient $[13]$, any significant strain $\varepsilon$ demands that the function $F(\theta)$ be large, of the order of $10^3$ to have a strain of a few percents. Hence $\dot{\theta}$, or $\varepsilon$, or both, must be in one of the two asymptotic regions $\theta \gtrsim 0$ or $\theta \lesssim \pi/4$. The threshold stress $\tau_c$ for grain sliding is generally in the range $0.5 \sim 5$ MPa, i. e. much smaller than the applied stresses $\sigma$ that are customary in mechanical tests. Hence the divergence at $\theta = 0$ should be the right one and appreciable strains occur for

$$\theta_c(\varepsilon, \dot{\varepsilon}, T) \approx 0.$$  

(15)

The other pole of function $F(\theta)$ corresponds to very slow flux, as occurring in superplastic deformation.

### D. Theory in the first order in $\theta_c$

Up to the first order in $\theta$ the expression in between the square brackets in Eqs. (11) and (13) reduces to

$$\left[ \frac{1 - \cos(2\theta)}{\sin(2\theta)} \right] - 2\theta \left( 1 + \frac{2}{\pi \sin(2\theta)} \right) - \frac{2}{\pi} \cos(2\theta) + \frac{\pi}{2} \right]^{-1}.$$  

(16)

The constant $\pi/2 - 4/\pi = 0.29756$ is not small enough and we can neglect $\theta$ when compared with it. Thus, with no significant lost of precision the exact equation

$$\frac{dp}{d\varepsilon} = sB \tau_c Q(p, T) \left[ \frac{1 - \cos(2\theta_c)}{\sin(2\theta_c)} \right] - 2\theta_c \left( 1 + \frac{2}{\pi \sin(2\theta_c)} \right) - \frac{2}{\pi} \cos(2\theta_c) + \frac{\pi}{2} \right]^{-1},$$  

(17)

can be reduced to the much simpler first order differential equation

$$\frac{dp}{d\varepsilon} = s \left( \frac{\pi - 8}{\pi} \right) C_0 B \tau_c \Omega^* \exp \left( -\frac{\varepsilon_0 + \Omega^* p}{k_B T} \right),$$  

(18)

whose solution can be written as

$$p - p_0 = \frac{k_B T}{\Omega^*} \ln \left[ 1 - C_0 \frac{\pi^2 - 8 \tau_c B}{\dot{\varepsilon} (\Omega^*)^2} \exp \left( -\frac{\varepsilon_0 + \Omega^* p_0}{k_B T} \right) \right].$$  

(19)

where it was substituted $\varepsilon_0 = |\varepsilon|$.

Eq. (19) expresses the main finding of this work: when the modulus $|\varepsilon|$ of the strain approaches from below the value

$$\varepsilon_{frac} = \frac{\pi \dot{\varepsilon}}{(\pi^2 - 8) C_0 \tau_c B} \left( \frac{k_B T}{\Omega^*} \right)^2 \exp \left( -\frac{\varepsilon_0 + \Omega^* p_0}{k_B T} \right)$$  

(20)

the hydrostatic pressure $p$ diverges logarithmically. According to the definition $[2]$ positive stresses (tension) contribute negatively to the hydrostatic pressure $p$. If the sample is conveniently annealed prior to the tensile test then $p_0 = -\sigma_0/3$, where $\sigma_0$ is the applied initial tensile stress. As the test proceeds, $p = -(\sigma + 2\sigma_\perp)/3$ increases monotonically with $\varepsilon$, and the transversal stress $\sigma_{\perp}$ increases from zero to negative (compressive) values. When $\varepsilon$ approaches the critical value $\varepsilon_{frac}$ the transversal stress $\sigma_{\perp}$ increases very rapidly, producing the characteristic neck and fracture. Therefore, Eq. (20) for $\varepsilon_{frac}$ expresses the strain to fracture of the material.

### E. Necking and strain to fracture

Eq. (20) gives the strain to fracture in terms of the constants of the theory. However one can express it in terms of more standard coefficients and easily measurable quantities. Combining Eqs. (5), (8), and taking into account the asymptotic approximation (15) to write

$$\cot(2\theta_0) + 2\theta_0 - \frac{\pi}{2} \approx \frac{1}{2\theta_0} \approx \frac{\sigma_0}{2\tau_c},$$  

(21)

Eq. (20) can be written as
\[ \varepsilon_{\text{frac}} = \frac{\pi}{(8 - \pi^2) \Omega^* \tau_c} \]  

(22)

We recall that \( \sigma_0 \) is the stress registered when the plastic deformation at the chosen constant strain rate \( \dot{\varepsilon} \) begins. The bulk modulus \( B \) is in tables and the only undetermined parameter is the product \( \Omega^* \tau_c \). However, \( \Omega^* \tau_c \) can be determined independently from other features of the plastic deformation of the sample in order to have a parameter free test of Eq. (22). To show how well this expression compares with experiment, we include next a study of a representative commercial steel.

Figure 2: Circles represent the stress–strain experimental data for a copper–alloyed high–strength interstitial free steel at the three strain rates shown in the inset [28]. The continuous lines represent the predictions of Eq. (11) with the parameters optimizing the fit to the experimental points, shown in Table I.

Table I: Values for the parameters giving the fits of Fig. 2 and calculated strains to failure.

| \( \dot{\varepsilon} \) [s\(^{-1}\)] | \( \frac{k_B \varepsilon}{\Omega^* B} \) | \( \tau_c \) [MPa] | \( \frac{\tau_c}{\sigma_0} \) | \( \varepsilon_{\text{frac}} \) |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| 200             | 8.03 \times 10^{-2} | 222             | 0.618           | 0.218           |
| 20              | 7.43 \times 10^{-2} | 208             | 0.667           | 0.187           |
| 1               | 1.06 \times 10^{-1} | 219             | 0.846           | 0.211           |

III. CONCLUSIONS

Although the existence of cracks and imperfections inside a stressed solid may contribute to accelerate fracture, the general cause of ductile fracture is not in them. An ideal fine–grained polycrystalline material, free of voids and cracks, whose grains are prone to slide, readily accommodating each other’s shapes, inevitably should fail after a finite plastic strain. The reason is an elementary condition that was advanced some years ago [19] but omitted in other studies: whatever the mechanisms for stress–dependent grain boundary sliding and grain shape accommodation may be, they must be consistent with density conservation to produce a steady flow. However, it is shown here that if the local shear stresses resolved in the planes of grain interfaces have a finite threshold for causing grain sliding, density is not conserved in the overall plastic flow. The grains are increasingly compressed as the sample is being stretched, and hence grain sliding can only proceed at the expenses of elastic volume variations of the crystallites. Fracture after a brief plastic strain, typically of a few percents, is a necessary consequence of the polycrystalline nature of the materials. The model gives a simple and precise closed–form equation for the strain to fracture, which is the strain at which the internal hydrostatic pressure diverges.

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