Preface

This module draws heavily on stuff dealt with in the next two chapters. Nevertheless it belongs into this chapter. See it as a taste treat of a science module and look at it again after reading the next two chapters.

Fracture Mechanics I

Energy Considerations

Calculating exactly why, when and how some material fractures is about the most difficult undertaking you can get involved with as a Material Scientist and Engineer. Since I never did that, and since the issue is quite complex, I can only look at some very basic principles here.

First, we consider the basic dogma of fracture mechanics:

Fracture occurs when cracks propagate. The cracks might have been there from the beginning or are formed under load.

This figure illustrates the basic idea:



Fracture occurs because unavoidable **microcracks** (better: **nanocracks**) that are always present at the specimen surface or inside the specimen, start to grow if the stress at the crack tip reaches a critical value. If cracks grow, they can do that very fast, roughly with the speed of sound. In the example above, where the specimen is under tensile stress, the crack tips would move roughly perpendicular to the applied stress direction. As soon as the crack tips start to move, fracture would be almost instantaneous - except if the conditions at the crack tip change, e.g. because the crack tip hits an obstacle and either stops or gets deflected.

So far this holds for brittle *and* ductile specimen. But of course there are major differences between the two. Ductile materials only fracture in a tensile test *after* extensive plastic deformation took place; look once more at the <u>typical</u> <u>stress-strain curves</u> and the figure below for the two extreme cases to appreciate that.



Note that as far as fracture is concerned, there is a big and obvious difference between *tensile* and *compressive* stress, in contrast to just <u>plastic deformation</u>. Tensile stress opens the crack, compressive stress closes it. That's why concrete or most "stones" can take enormous compressive stresses, e.g. at the base of Khufu's (Cheops) pyramid, but fail quickly under tensile loads. The solution to this problem is re-enforcing you concrete with steel that can take the tensile stress.

Let's first look at a quite general fracture model. We ask ourselves *why* crack tips do not start running already at low stresses. Why do specimen as shown above do not break immediately, if stressed? That is not a simple question. So let's look at the most simple (haha) case first: Let's fracture an *ideal perfect brittle crystal* with no nanocracks and so on. We know that we can fracture anything, even an ideal crystal, because the <u>First Law of Materials Science</u> always applies.

The <u>spring model of crystals</u>, where you consider the bonds between the atoms to behave like little springs, gives an easy-to-calculate first answer. Well, not quite that easy but not too difficult with a few well-chosen approximations. What we do is to simply calculate the total work or *energy* needed to pull out the bond-springs between the atoms to a large distance, effectively fracturing the crystal. In the link above that's done with a lot of math, but the <u>result</u> doesn't get us very far. The reason is that in this model we fracture *all* the bonds in one fell swoop, whereas in reality we fracture them "one-by-one" as a crack grows - and that is considerably easier. The decisive insight comes from asking a simple question:

A lot of energy is needed to fracture a material. Where does this energy go?

You have invested a lot of work for destroying a piece of crystal by ripping it apart. Where is that energy now? Energy, after all, is <u>conserved</u>. It cannot simply disappear.

One might guess that the fracture energy will turn to heat, making the two fractured parts somewhat hotter. It does that, allright, but that is only a minor side effect. Most of the energy, as **Alan Arnold Griffith** first realized, is needed to create the two **new surfaces** that did not exist before fracture.

Surfaces, or more generally *interfaces*, possess some <u>surface energy</u> of their own. Atoms in an interface like the surface are not as happy as atoms in the interior of a perfect crystal, where they have exactly the environment they like best. That means that this environment has the <u>smallest (free) energy</u> by necessity. By default, any environment different from that of a perfect crystal must have a higher energy. Chapter 4 and chapter 5 deal with this in detail.

OK - enough foreplay now, time to start the serious stuff.

If we calculate the energy needed to rip some of the bonds of a perfect crystal apart, and equate that with the energy needed to generate the new surface, we obtain a rather simple (approximate) equation:



We already know the meaning of most symbols, the rest are easy:

- 1. σ_{crit} is, of course, the critical or maximum stress one can apply. Go a smidgen above σ_{crit} , and instantaneous fracture occurs.
- 2. **Y**, as always, is <u>Young's modulus</u> and thus (as we are going to <u>learn soon</u>) a measure of the "strength" of the bonding springs.
- 3. *a*₀ is simply the distance between the atoms, roughly around **0.3 nm**.
- 4. γ is the specific energy of the surface (measured, e.g., in **J/m²**) and thus a quantity that can be measured or calculated.

The meaning of the equation is just as easy to see:

- For the materials under consideration, get the three numbers for the three quantities on the right hand side. That is not difficult, most of that stuff is known and recorded somewhere.
- Multiply Y and γ, divide by a₀, take the square root and you know the maximum stress your *brittle* material can take without fracturing.

Or do you? No, you don't. Any material you like to test will fracture at much smaller stresses than the one calculated above. Not just a little bit smaller, but 10 or 100 times smaller! Worse, the fracture stresses measured for nominally identical materials, while always much smaller than the calculated one, are often wildly different.



Without reliable numbers for the stress a material can take, there is no reliable design or construction of mechanical machines. True, we do not built airplanes and so one from brittle materials, but the situation for *ductile* stuff like aluminum alloys is not much better as we shall see.

And yes, the problem has been solved throughout the millennia by simply making the mechanically challenged parts of a construction far bigger than absolutely necessary. If your new temple collapsed because the columns (brittle material!) fractured under the weight, you made them bigger and bigger. Same thing for *early* metal constructions: they were rather solid and not given to fracture. *Later* metal constructions like early railway stuff and steam boilers fractured like crazy, killing lots of people. So good steel was invented and heavy parts were made. Problem solved once more. Well, yes, but those things wouldn't *fly* - far too heavy.

There is a need to make light-weight constructions that can fly, go very fast (like non-American trains), do not break apart in cold water (like some <u>American ships</u>), or get very high mileage (like non-American cars). If you want to do this, you depend rcompletely on *reliable* numbers for what the material can take - in terms of critical loads and many other parameters.

The reason for premature fracture, as *Griffith* first realized, are tiny defects in the materials, in particular something Griffith called *microcracks* and that I will call *nanocracks*, because it causes already sufficient trouble if those defects are in the nanometer range. Nanocracks (and other defects) are always present in *real* materials. Griffith didn't just realize the relation between fracture and defects, he performed interesting calculations, getting extremely important results.

To get a taste treat of what Griffith did, let's now look at a sample under tension as above, but with a nanocrack as shown below in some more detail.

The first thing to realize is that a roughly circular area (in three dimensions it would be a cylinder) around the nanocrack (darker blue) is more or less stress-free. Just imagine the light blue part below to be a rubber band with a slot and you see what I mean. Since "nobody" pulls at the already fractured part, there cannot be much stress there.



Iron, Steel and Swords script - Page 3

Very roughly, the area inside the blue circle with a radius *d* = half width of the crack is stress free since "nobody" pulls at the atoms at the surface of the crack. In reality, the stress increases gradually from zero at the crack surface to the bulk value with increasing distance from the crack.

Maximum stress occurs at the edges of the nanocrack. The stress state there is not <u>uniaxial</u> as in the bulk of the material but more <u>complicated</u>. Whatever, rather similar energy arguments as for fracturing an ideal crystal apply:

- Growth of the nanocrack generates new surface and that "costs" surface energy γ .
- Growth of the nanocrack generates a larger stress-free region and that releases or "pays" elastic energy fewer <u>bonding-springs</u> must be elongated.

Crack growth thus is only a good energy investment for a crystal if more elastic energy is released than needed for increasing the surface. The equation resulting from working that out is called **Griffith criterion**; here it is:

$$\sigma_{\text{crit}}(\text{real}) \approx \left(\frac{2Y \cdot Y}{\pi d}\right)^{1/2}$$

- This is pretty much the same (approximate) equation we had for the perfect ideal crystal <u>right above</u>, *except* that the distance **a**₀ between the atoms is replaced by the half-width **d** or about the size (see the figure) of the nanocrack! And never mind the $(2/\pi)^{\frac{1}{2}} = 0.8$; it just appears because I need it later. All this is approximate, anyway, and a factor of **0.8** is close enough to **1** to be of no importance here.
- What that means is obvious. A crystal containing just one nanocrack with a width of, for example, 2d = 60 nm (or roughly 25a ₀), will fracture at roughly 1/5 of the stress needed to fracture an absolutely perfect crystal. Consider that a 60 nm nanocrack is far too small to be seen with the best optical microscopes, and that a surface containing nanocracks of this size would still look well polished. The message is clear:



Stress Considerations

Looking at the total energy of a large system is always a good thing to do. It will tell what the system as a whole is apt to do. It's like looking at national economics. The guys looking into this will tell us how the economy of the country could benefit if some extra money would float around and we all do the right thing with it. On the other hand, if your wife will come into possession of some extra money, chances are that she will neither know nor care about what would be good for the national economy, but dispose of the windfall in any way she likes.

Nanocracks are no better than your wife you. They neither know nor care about what would be good for the total energy of the crystal. All they know is that in order to move, they must break the bonds between the atoms right at the crack tip. The figure below illustrates that.



Shown is *strain*. The larger the distance between atoms on top of the equilibrium distance, the larger the strain. Since the strain is proportional to the stress, it is essentially the same thing.

As soon as the stress at the crack tip is large enough to rip apart the bonds between the atoms there, the crack tip will move. The crack gets larger and the crystal fractures. No atom there gives a damn about surface energies, etc. What we must do now is to calculate that stress.

That's not an easy job since the stress at the crack tip is not uniaxial as in the bulk of the crystal but more <u>complex</u>. Nevertheless, in a good approximation, the stress σ_{tip} at the crack tip for a uniaxial situation as shown can be calculated to

$$\sigma_{\rm tip} \approx 2\sigma_0 \left(\frac{d}{r}\right)^{1/2}$$

 σ_0 is simply the nominal tensile stress acting on the specimen; *d* is the half-width of the crack as before, and *r* is the radius of a sphere that one could inscribe at the crack tip and that measures how acute or blunt the crack tip is. This is illustrated below.



- In any case, the stress at the crack tip is larger than in the bulk of the material, an effect called stress concentration. At a sharp tip (small radius *r*) the stress is larger than at a blunt tip (large radius *r*). The crack thus will start moving at lower loads than at the blunt tip.
- Is that contradicting the earlier energy consideration? Not at all. Like in national economy, the things that are predicted on the large scale come about without direct consideration of what is going on at the small or individual scale. If we look at the small scale (atoms) or large scale (energy of zillions of atoms) is simply a matter of convenience.

We have almost all the major ingredients now to understand the basic principles of fracture in brittle and ductile materials. What's missing is the basic principle behind *ductility*.

- In other words: What happens if *plastic deformation* occurs? In yet other words: What other kinds of defects besides nanocracks do we have in crystals and how is all of that connected? We must know a bit about that before we can go on.
- So read <u>chapter 4</u> and <u>chapter 5</u> of the backbone now.

To be continued.
