3.2.3 Stress and Strain

Thermal Stress and Strain

- You have made a **200 nm SiO_2** layer on you **100 mm x 100 mm Si** substrate (it is easier to consider it to be it square here) with some process at **1.000 K** and now you cool it down to room temperature (**=300 K**).
  - **SiO_2** on **Si** is one of the most frequently made thin layers. But you will find that you now have a tremendous stress in your **SiO_2** film.
  - The same is true for pretty much any thin film made at a temperature different from room temperature.
  - The question coming up now is obvious. *Why* stress, and *how much* stress?
- The "*why*" is easy. Upon cooling, substrate and thin film will shrink by some factor given by their **thermal expansion coefficient** α, a property we have encountered before and seen that it comes straight from the bonding potential.
  - The thermal expansion coefficient α was defined as

$$\alpha = \frac{l(T) - l_0}{l_0 \cdot T} = \frac{\epsilon_{therm}}{T}$$

  - l_0 is the length at the reference temperature, usually room temperature. Of course, α might be a function of the temperature; more generally we would define it as $\alpha(T) = d\epsilon_{therm}/dT$.
- It follows that two different materials with an α_A and an α_B, having the same length l_0 at some T_0, will differ in length at the temperature T by some $\Delta l(T)$ directly proportional to the **mismatch in the thermal expansion coefficient** and given by

$$\Delta l(T) = l_0 \cdot \Delta T \cdot (\alpha_A - \alpha_B)$$

  - Dividing $\Delta l(T)$ from above by l_0 obviously describes a strain ϵ_{TF}. The subscript "TF" stands for "Thin Film" since the strain (and the stress) will occur almost exclusively in the thin film, as explained below. We have

$$\epsilon_{TF} = \Delta T \cdot \Delta\alpha$$

- Let's suppose that we cover a **100 mm** Si wafer with some oxide ar **700 ^oC**. What happens when we cool down?
  - Fierst we need numerical values for α, which we can easily find - Wikipedia, for instance, gives us
    - $\alpha_{Si} = 3 \cdot 10^{-6}\ K^{-1}$
    - $\alpha_{quartz} = 0.6 \cdot 10^{-6}\ K^{-1}$

    More values are given in the link
  - Taking these numbers we get:
    - $\Delta l(T)_{Si} = 100 \cdot 700 \cdot 3 \cdot 10^{-6}\ mm \cdot K \cdot K^{-1} = 0.21\ mm$
    - $\Delta l(T)_{SiO2} = 100 \cdot 700 \cdot 0.6 \cdot 10^{-6}\ mm \cdot K \cdot K^{-1} = 0,042\ mm$
  - In words: The **Si** substrate would like to be **0,17 mm** smaller than the **SiO_2** layer after cooling down to room temperature.
  - However, since **SiO_2** adheres very strongly to **Si**, both materials must have the *same* lateral size and there is now a contest of strength. The Si tries to pull the **SiO_2** layer to a smaller size, the **SiO_2** layer pulls back, trying to keep the **Si** larger then it wants to be.
  - There can be no doubt about who will be the winner. Since there is far more **Si** than **SiO_2**, silicon "wins" and the **SiO_2** layer is simply forced to shrink more during cooling than it would like to.
  - The **SiO_2** thus is forced to the same lateral size as the **Si** substrate and builds up compressive stress that produces a "shrinkage" of just **0.2 mm** at room temperature. It will be under compressive stress, in other words.
- We can generalize to all thin films: A difference $\Delta\alpha$ of the thermal expansion coefficients between substrate and thin film material and a temperature difference ΔT relative to a stress few state produces a strain $\epsilon_{TF} = \Delta T \cdot \Delta\alpha$ in the thin film.
  - If that strain is purely elastic, it will lead to a stress σ_{TF} in the thin film given by

$$\sigma_{TF} = Y \cdot \epsilon_{TF} = Y \cdot \Delta T \cdot \Delta\alpha$$

- Y is, of course, ***Young's modulus*** ("Elastizitätskoeffizient").

Once more: why is the stress in the thin film? Well, you try to sit atop a huge steel bridge and stop its thermal expansion relative to yours by pulling hard. You are not going to win, neither is a thin film on a thick substrate. However, this is only true up to a point that we will discuss below.

- For our example we get with Y_{quartz}**=70 GPa**

$$\sigma_{quartz} = 70 \cdot 10^9 \cdot 0.2\ \text{mm} / 100\ \text{mm} = 140\ \text{MPa}$$

- This is a lot of stress! It means that you have to press on the tiny cross section of $(100 \cdot 2{\cdot}10^{-4})\ \text{mm}^2 = 2{\cdot}10^{-2}\ \text{mm}^2$ of our thin film with a force $F = 147{\cdot}10^6\ \text{N/m}^2 \cdot 2{\cdot}10^{-8}\ \text{m}^2 = 2.94\ \text{N}$.

Stress Relaxation Mechanisms

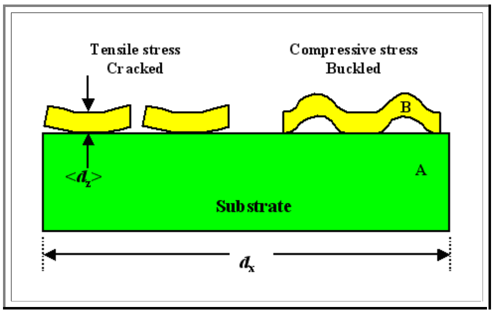
Now let's generalize some more: We know now that if we change the temperature of a substrate - thin film system, we generate stress. We also know now that we might generate a *lot* of stress.

From before, we know that no material will be able to sustain arbitrarily large amounts of stress without something happening. We now ask: What is going to happen? How will the stress in a thin films be relieved, or, to use the common expression: what are the mechanisms of *stress relaxation*?

There are many "easy" answers *in general*. Unfortunately, the answer for your particular system may not be easy to obtain. Let's look at some special cases:

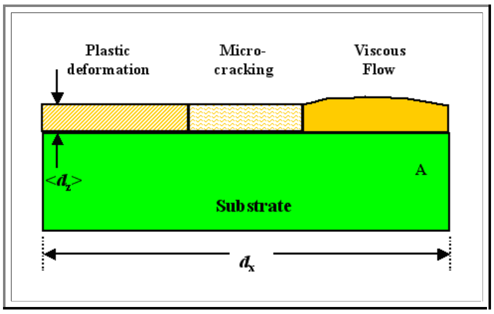
1. The adhesion is not very good.

- If your adhesion is not very good, your film may simply come "loose" - in total or in parts. Wherever it does not adhere to the substrate anymore, the stress can be completely relieved.
- The criterion, as always, is that if the energy gained by stress relieve (=½ σ · ϵ per volume times thickness) is larger than the interface energy, it "pays" to rip off. Obviously, this scales with the film thickness.
- The problem is that the energy balance of a mix of partially coming off, partially still sticking, is not that easy to calculate. First you have to consider if you have tensile or compressive stress, and then what additional energy terms come into play
- **Fracture** or cracking in the tensile stress case, or "**buckling**" in the compressive stress case, also takes some energy. What you will get thus depends on many things. But whatever you get - *you probably won't like it!*



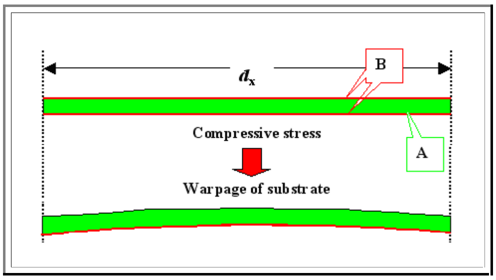
2. The adhesion is very good - the interface does not "give". This means that you will find a fully adherent thin film *and* still a lot of stress. But not necessarily the full stress you would calculate!

- There are some stress relieve mechanisms without the layer coming off that may become activated and reduce the stress in your thin film.
- Most simple, of course, is plastic deformation if your thin film is crystalline. As soon as you exceed the ***critical yield strength*** or shear stress, you will get plastic deformation. **Dislocations** will move; if too few are present, some will be generated.



- However, for plastic deformation to occur, at least one of your two materials must be ductile and not brittle. At this point it is important to note that perfectly brittle materials at room temperature (like **Si** or **Ge**) might be quite ductile at high temperatures. Note that some plastic deformation may also occur in the substrate.
- If your thin film is brittle at all temperatures, it might "microcrack", whatever that means. The link provides some insights into the some puzzles investigated right now in this context.
- In the case of our example from above, where we have produced *amorphous* $\mathbf{SiO_2}$, plastic deformation by dislocation movement is impossible by definition. We might have plastic deformation by **viscous flow**, however.
- In fact, amorphous $\mathbf{SiO_2}$, being a glass, is somewhat viscous at our chosen temperature of **1.000 K**; and some of the stress generated during cooling down will be relieved

Whatever happens, chances are that you will have some appreciable stress left after cooling down because the stress in the this layer could not be fully relaxed. We now give a quick glance of what might happen to the substrate in this case.



- Now me must look at little bit closer on how we made the thin layer. In the example from above it would have been thermal oxidation - we simply stick the **Si** wafer in a furnace at **1.000 K** with pure $\mathbf{O_2}$ inside. An $\mathbf{SiO_2}$ layer will grow in essentially the same way as a rust layer grows on iron. We look at this quite closely in the context of making **IC's**.
- The thing to realize here is that we do not just get an oxide layer on the wafer surface, we get exactly the same one on its backside. Whenever you make a thin layer, you always must ask yourself from now on: Will it grow just on one side or on both sides? What would be better?
- But now you have an oxide layer, being under considerable compressive stress, on both sides. Otherwise your square of **Si** looks perfect.
- Clearly, if you want to make an *integrated circuit*, you don't want or need an oxide layer on the backside. So you take the backside layer off - stick it in hydrofluoric acid (**HF**) for example, with the front side protected by some layer of wax you painted on.
- Big mistake! Now your whole substrate will be warped - you have just encountered the phenomenon of "**warpage**".

Warpage can be a serious problem in thin film technology. The reason for it is clear. Your thin film exerts a two-axial normal force on any pixel of your substrate, and your substrate will respond somehow.

- If it doesn't deform plastically (not possible for e.g. **Si**, ceramics, and so on) it will respond by elastic deformation. It may not respond a lot, but respond it will.
- For a (round) wafer with thickness d_A and Young's modulus Y_A, on top of which a thin film with thickness d_B has been deposited, that is under a stress σ_A, we can make an easy educated guess of what we would find for the **radius of curvature** R. Remember: R is *small* if the wafer is heavily warped, and *large* if it is almost flat.
- What we must expect is
  - $R \propto 1/\sigma_A \cdot d_B$ because $\sigma_A \cdot d_B$ gives the force bending the wafer.
  - $R \propto Y_A$ because Y_A is a measure of how much the substrate will "give" for some force.
  - $R \propto d_A{}^2$ because the bigger d_A the less it will bend. That R is proportional to the square of d_A may not be obvious right away (the "Wolf and Tauber", by the way, give a wrong equation without the square), but a radius of curvature in this case is necessarily defined in two dimensions, so we must have $d_A \cdot d_A$.
  - R must not depend on $d_{x,\,y}$ because for a radius of curvature this dimension doesn't matter - at least as long as $d_{x,\,y} >> R$.
- What we will get by really deriving the radius of curvature R by going deep into elasticity theory is the "**Stoney**" **formula** (cf. e.g. "Ohring" p. 727).

$$R = \frac{1}{6\sigma_A \cdot d_B} \cdot \frac{Y_A \cdot d_A^2}{(1 - \nu)}$$

- So, besides ν, ***Poisson's ratio*** coming in (as always when considering two-dimensional elasticity problems), with **1 – ν** coming out to an almost negligible ≈ **0.7**, the only thing we missed is the factor **1/6**.

One thing we can learn already here. When we consider **IC** technology we will see that we make a lot of layers on the **Si** backside, where we don't need them. We will take those layers off - but at the exactly right moment in time, when we can afford to loose the "counterbalance" they offer in terms of stress and strain management.

Stress and Strain in Thin Films Not Coming From Temperature Differences

You do not necessarily need a temperature difference to generate stress in your thin film. Your method of depositing or making the thin film may already produce *intrinsic* stress and strain.

Since there are many different ways to produce thin films, we will not go into details here. We will just look into two extreme cases:

- **1.** Producing stress is an integral part of the film generating method. This is true, for example, if the thin film is produced by a chemical reaction with the substrate. The paradigmatical example is **Si** oxidation as outlined above, where a certain volume of **Si** is converted into a different volume of oxide (almost twice as large). This is just not possible without generating considerable stress.
- **2.** The stress produced is a function of many parameters. You may or may not understand the exact relationship between your deposition parameters and the stress produced, but you may now start to optimize. Note that you do not necessarily want stress-free layers. What you want is control!

The long and short of this paragraph is a simple message:

Stress management is an integral part of thin film technology