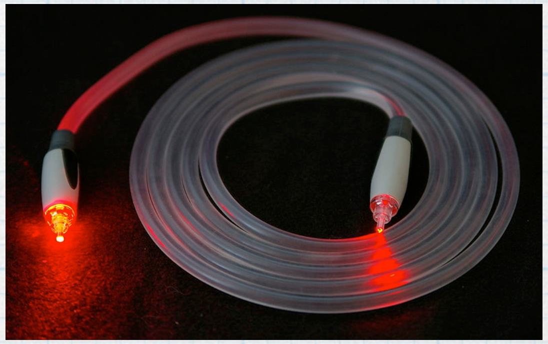
Silicon dioxide, SiO_2

Sand (silica) – one of the most common minerals in the earth.

Main component in common glass

- mixed with sodium carbonate and calcium oxide (lime) to make soda-lime glass for window panes, bottles, drinking glasses, etc.

Main component in optical fibers



Crystalline SiO_2 is *quartz*

- fancy drink ware and artwork
- crystal oscillators using the piezoelectricity)
  http://en.wikipedia.org/wiki/Crystal_oscillator
- Laboratory equipment

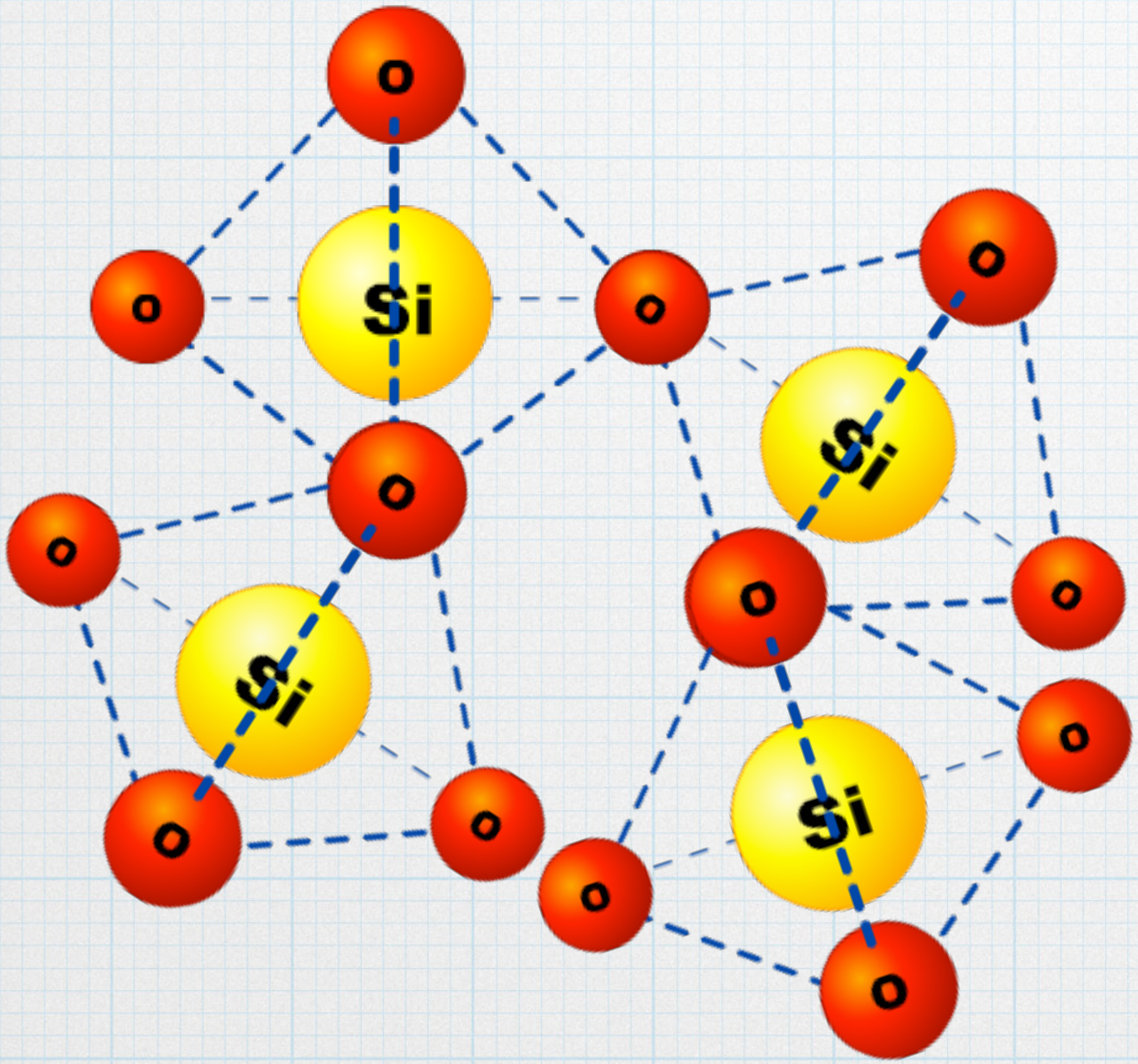
Food additive (?!)

Microelectronics

- thin electrical insulator (MOSFET gate)
- diffusion barrier

SiO_2 structure

Tetrahedral arrangement with one silicon bonded to four oxygen atoms.



Most oxygen atoms will be bonded to two silicon atoms, so that two tetrahedra are joined at a corner. (bridging atoms)

The orientation can be random, leading to an amorphous structure. Some oxygen atoms will be bonded to only one silicon atom (non-bridging atoms). The relative amounts of bridging to non-bridging determines the "quality" of the oxide.

If all oxygen atoms are bridging, then a regular crystal structure results – quartz.

SiO_2 properties

- In microelectronics, we use thin layers of pure SiO_2. The layers are amorphous (fused silica)
- Density: 2.0 - 2.3 gm/cm^3
- Dielectric constant at low frequencies: $\varepsilon_r = 3.9$ (remember this!) refractive index at optical wavelengths: $n \approx 1.5$
- Breakdown field: > 10^7 V/cm (1 V across 1 nm)
- The interface with silicon always results in electronic trap levels and some negative interface charge. Typical interface defect density ≈ 10^{11} cm^{-2}. This is not a high density of defects at an interface. It can be made even lower by annealing in hydrogen.

The combination of the relatively good electrical properties of silicon, the excellent insulating properties of SiO_2, and the low-defect interface between them is the key ingredient of modern integrated circuit electronics.

Oxidation of silicon

There are several ways to form a layer of SiO_2 on the surface of silicon. The two pre-dominate methods are:

- Thermal oxidation of silicon - react silicon from the wafer with oxygen to create oxide.
- Direct eposition of a thin oxide film by chemical vapor deposition. (We'll discuss this in detail later.)

Thermal oxidation is a simple process - introduce an oxidizing atmosphere to the surface of the silicon with sufficient temperature to make the oxidation rate practical. There are two commonly used variants:

- Pure oxygen: $Si + O_2 \Rightarrow SiO_2$ (dry oxidation)

- Water vapor: $Si + 2H_2O \Rightarrow SiO_2 + 2H_2$ (wet oxidation)

Typical oxide thicknesses range from a few nanometers to more than 1 micron. The details of the process and a mathematical model are presented in the next lecture.

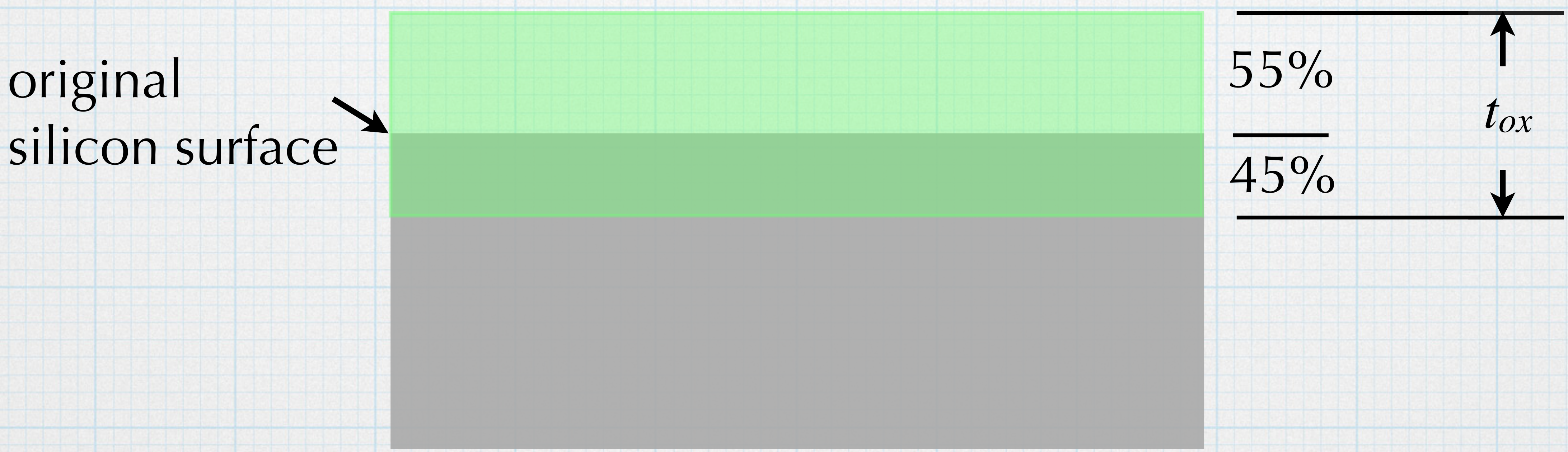
Consumption of the silicon substrate

- In the reaction forming SiO_2, silicon atoms at the surface of the wafer combine with oxygen and are incorporated into the oxide film. For a given volume of SiO_2 that is formed, a corresponding volume of the silicon substrate is lost.

- In crystalline silicon, each silicon atom corresponds to a volume of 2×10^{-23} cm^3 (= 0.02 nm^3). In SiO_2, each silicon atom corresponds to a volume of about 4.4×10^{-23} cm^3, depending on the density of the oxide, or about 2.2 times more than the volume in the silicon.

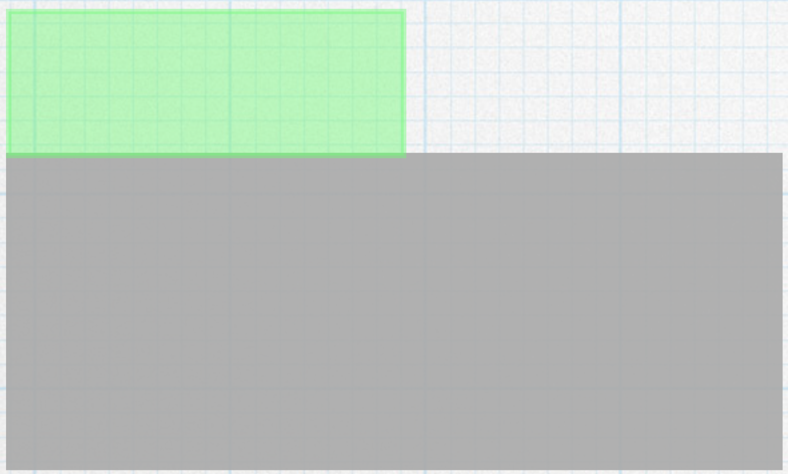
- However, as the SiO_2 is forming, it cannot expand in all directions equally – it is constrained in the plane of the wafer. So all of the volume difference is taken up by expansion in the vertical direction.

Thinking about this in reverse, for a given thickness of oxide, t_{ox}, the fraction of the thickness that corresponds to consumed silicon is 1/2.2 or 0.455. So, in growing the oxide, $0.455t_{ox}$ of the final silicon dioxide thickness corresponds to silicon that was "lost". The grown oxide extends an additional $0.545t_{ox}$ above the original surface of the silicon.

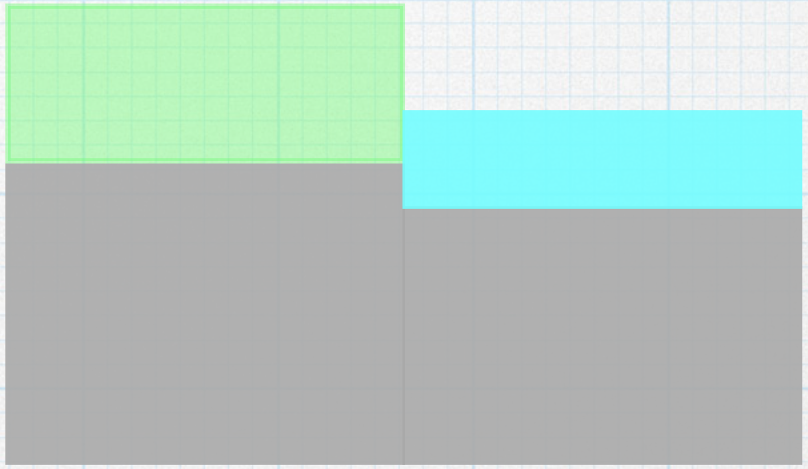


Steps at the surfaces and interfaces

Grow an oxide layer. Then pattern and etch away the exposed region.



Then grow a second oxide layer. The oxide in the exposed region grows faster than in the other area.



Steps are created at both the oxide surface and the Si/SiO_2 interface.