3.3 General Device and Product Considerations

3.3.1 Interfaces and Contacts

This Module is unfinished

General Remarks

- Practically all **Si** devices and all other solid state devices have properties that are "*interface controlled*".
  - The "**pn**-junction" is an interface and so is the **MOS** contact. The latter, in fact, involves two interfaces: **Si**-oxide and oxide-metal. But there are many more interfaces: Metal-**Si** contacts are needed to connect the device to the outside world and there are many interfaces between the various layers in integrated circuits.
  - What kind of interface properties do we want to have? This is not a simple question: In the case of the **pn**-junction we certainly want the "**metallurgical junction**" (the area of actual contact between the **p** and **n**-type Si) to have *no structural properties* - it should be impossible to find it analytically as far as the **Si** is concerned. Of course, the metallurgical junction of a a **pn**-junction formed by diffusion is not really definable; but you also could make a **pn**-junction by epitaxy and then the metallurgical junction is wherever the surface of the substrate *was*.
  - On the other hand, it would not be too far fetched to assign all the *electronic properties* of a **pn**-junction to the interface (one certainly would do this for a metal-metal junction).
- Usually we would like a metal - **Si** contact to be *ohmic* - and not of the Schottky type. This again might be seen as an interface property. For both electronic properties mentioned we would like them to be as independent from structural properties as possible. In other words, the precise arrangement of the atoms in the interface, the presence of interface dislocations, etc., should not matter much.
- Then we have structures where we hope that the interface does not have any properties relevant to the device function.
  - Interfaces for a **MOS** contact, e.g., are not really required for the function - theoretically we could remove the dielectric and run the device in vacuum with somewhat changed parameters because of the changed dielectric constant. The question now is if there are interface properties that interfere with the device operation.
  - We certainly would tend not to worry about the properties between some insulating dielectric layers or call for "no" properties - but that is not correct, we definitely want that the stick together solidly, or, in other words, we want some bonding or adhesion.
- We thus must ask ourselves: What are the properties an interface can have and how do those properties influence or even enable device operation.
  - What are the basic properties an interface can have?
  - What is the variation range of a given property and how can it be influenced or tuned to specific needs?
  - How do specific properties interact? For example, how does the atomic structure correlate to electronic properties, e.g. states in the band gap?
- Looking at interfaces in this kind of generality, we are opening a rather big can of worms. However, we will stay short of the more structural considerations and focus on just a few examples with some importance to semiconductor devices.

Properties of Interfaces

- First, we restrict ourselves to properties that are directly linked to the interface; i.e. that stem from whatever the interface introduces *locally*. Interface states in the band gap are an interface property in this sense, but not the space charge region of a **pn**-junction, or the junction properties themselves.
  - In principle, all these properties are then given by the exact structure of the interface, i.e. the exact location of all atoms and their interaction with their neighbors, i.e. the bonding situation.
  - We may distinguish between intrinsic and extrinsic properties. *Intrinsic* properties result from an interface between two "ideal" materials that do not contain unwanted impurities - in other words we look at a "perfect" interface. Note that perfect interfaces may still contain lattice defects, e.g. so-called grain boundary dislocations, as an intrinsic part of their structure.
  - *Extrinsic* properties result from the incorporation of impurity atoms, precipitates and other structural defects not present in the intrinsic case.
- Looking at an (incomplete) list of interface properties, what comes to mind are the following topics:
  - **Interface energy**. A few numbers give an idea of the magnitudes encountered:
    - Coherent twin boundary in **Si** (smallest interface energy for **Si** grain boundaries): ≈ **60 mJ/m^2**
    - General grain boundary in Si: ≈ **600 mJ/m^2**
    - Silicon - **SiO_2** interface ???

- **Interface "Strength"**: How much energy (or mechanical stress) is needed to rip the two materials apart? Looking at the many interfaces of a typical integrated circuit this does not appear to be a problem - the whole thing sticks together pretty well, However, this is more a lucky accident. If you try to to replace the intermetal dielectrics (usually some variant of **SiO_2**) with some kind of **CF_4** (Teflon in other words), you will have big problems because it does not "stick". And you would dearly love to use Teflon for modern high speed devices because it is one of the few eligible materials with a very low dielectric constant. Of course, interface strength is related to the interface energy.
- **Interface structure**: There are several layers of complexity when considering the interface structure:
  - First, you may have to ask yourself if you really have a "simple" **A-B**-interface. On a more macroscopic (but intrinsic) level you may wonder if there is an intermediate layer - e.g. a thin amorphous layer of some **Si - N**i mixture between a **Si - $NiSi_2$** interface, to give an example (there isn't, by the way), or if there is an abrupt crystalline - amorphous transition at the **Si - SiO_2** interface or gradual loss of crystallinity in the **SiO_2** interface (it's rather abrupt), or if there are any preferred crystallographic orientations for interfaces between crystals (there usually are), and so on
  - For crystalline - crystalline interfaces you may ask next, if there are any intrinsic structural units, e.g. networks of dislocations (e.g. grain boundary dislocations or misfit dislocations).
  - Yet a level down, the question will be how an interface deals with intrinsic lattice defects, e.g. dislocations impinging on it, steps in the interface plane or changes in the plane of the interface (the interface may be bent, after all)
  - Finally, you have to consider the influence of extrinsic components. Point defects might segregate at the interface and even form precipitates, or small highly mobile atoms (usually **H**) may become stuck at the interface (bonding to "**dangling " bonds**, i.e. bonds that are nit saturated.

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- **Interface "chemistry"**: Interfaces are often more reactive in a general sense of the word than the bulk material. Corrosion, in particular, may not only proceed along interfaces much more rapidly than in the bulk; it may be caused by the "galvanic" properties of the interface, Somewhat more general, diffusion of atoms or molecules might be quite different in interfaces than in the bulk.
- **Interface charge:** Interfaces might be charged for a variety of reason, and this brings us closer to the more interesting properties for semiconductor devices:
  - It is almost impossible to balance charges exactly in interfaces between ionic crystals or materials with some ionic binding component. The interface then carries a net charge that is balanced either by other parts of the interface, by charged point defects, or by other interfaces. The charge is felt for a distance of about a Debye length; in all conducting media it is therefore hardly noticeable. This is an essentially *intrinsic charge*.
  - If the interface has some energy states in a bandgap, these states may or may not be occupied by electrons, depending on the Fermi energy of the system. The interface therefore may carry some variable amount of charge. Again, this is essentially an *intrinsic charge*.
  - If some *extrinsic* ions are solidly trapped in the interface - e.g. alkali metals and ***alkaline earth*** metals like **Na**, **K**, **Ca**, etc. in the **Si - SiO_2** interface - there will be some charge in the interface too. This then is an *extrinsic charge*

  Some devices, e.g. ***EPROM***s, rely on interface charge - and on the fact that it may stay there for very long times!
- **Interfaces states** - for electrons or holes. While the density of states is always affected by interfaces, they must not necessarily introduce energy levels in the band gap; i.e. only the density of states in the valence and conduction band may be affected.

Reactive and Non-Reactive Interfaces

- Whenever we make an interface between materials **A** and **B** by depositing **B** somehow on **A**, the formation of the final structure with all its properties will occur between two extreme cases
  - For a *non-reacting interface*, the **B**-atoms just stay pretty much wherever the are deposited.
  - For a *reactive interface*, interdiffusion takes place, forming some **A-B** mixture or even defined compounds **A_x B_y**.
- Non-reactive interfaces usually become reactive to some extent upon heating.

Topics to be covered

Si-SiO_2 Interface, Si - metal, silicides