1.3.2 Materials Properties and Defects

Material Properties and Defects

- Defects determine many properties of materials (those properties that we call "structure sensitive properties"). Even properties like the specific resistance of semiconductors, conductance in ionic crystals or diffusion properties in general which may appear as intrinsic properties of a material are defect dominated in case of doubt by the intrinsic defects. Few properties e.g. the melting point or the elastic modulus are not, or only weakly influenced by defects.
- To give some flavor of the impact of defects on properties, a few totally subjective, if not speculative points will follow:
 - Generally known are: Residual resistivity, conductivity in semiconductors, diffusion of impurity atoms, most mechanical properties around plastic deformation, optical and optoelectronic properties, but we also have:
 - Crystal growth, recrystallization, phase changes.
 - Corrosion a particularly badly understood part of defect science.
 - Reliability of products, lifetimes of minority carriers in semiconductors, and lifetime of products (e.g. chips). Think of electromigration, cracks in steel, *hydrogen embrittlement*.
 - Properties of quantum systems (superconductors, quantum Hall effect)
 - Evolution of life (defects in DNA "crystals")
- A large part of the worlds technology depends on the manipulation of defects: All of the "metal bending industry"; including car manufacture, but also all of the semiconductor industry and many others.

Properties of Defects

- Defects have many properties in themselves. We may ask for:
 - Structural properties: Where are the atoms relative to the perfect reference crystal?
 - Electronic properties: Where are the defect states in a band structure?
 - Chemical properties: What is the chemical potential of a defect? How does it participate in chemical reactions, e.g. in corrosion?
 - Scattering properties: How does a defect interact with particles (phonons, photons of any energy, electrons, positrons, ...); what is the scattering cross section?
 - Thermodynamic properties: The question for formation enthalpies and -entropies, interaction energies, migration energies and entropies, ...
- Despite intensive research, many questions are still open. There is a certain irony in the fact that point defects are least understood in the material where they matter most: In <u>Silicon!</u>

Goals of the course

- This course emphasizes structural and thermodynamic properties. You should acquire:
 - A good understanding of defects and defect reactions.
 - A rough overview of important experimental tools.
 - Some appreciation of the elegance of mother nature to make much (you, crystals, and everything else) out of little (92 elements and a bunch of photons).