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 Silicon!

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).