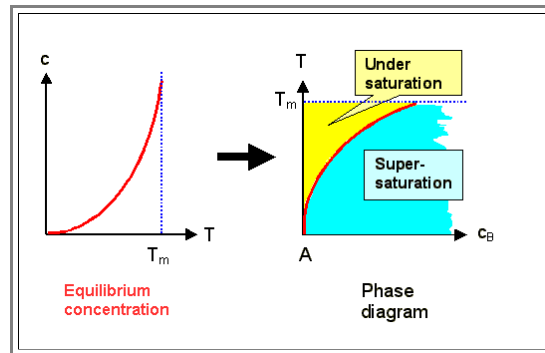


Phase Diagrams

Basics

Phase diagrams are the mainstay of materials science and technology. They may be seen as a *map* in temperature - composition space that shows the particular structure with the minimum free enthalpy at any point of the "map".

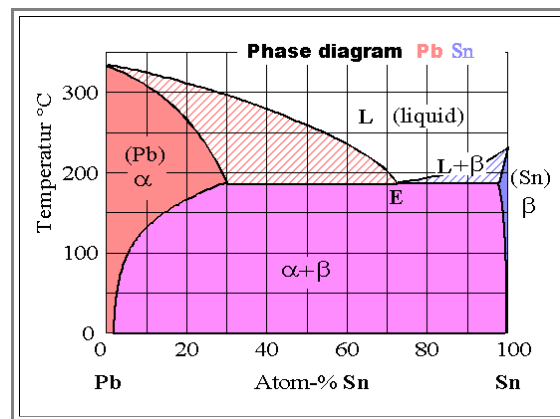
- If we take the [formula for the equilibrium concentration of self-interstitials](#) to also describe the equilibrium concentration of extrinsic interstitial atoms if we replace the formation enthalpy by a corresponding property (lets call it *solubility enthalpy*), the resulting diagram of the equilibrium concentration over temperature can be interpreted as part of a phase diagram.
- All we have to do is to switch the axes from the normal representation *concentration vs. temperature* to *temperature vs. concentration*:



We now have a diagram for the composition of material **A** (the matrix) with material **B** (the extrinsic interstitial) for small concentrations of **B**.

- The red line denotes the limit of solubility of **B** in **A**; it corresponds to the equilibrium concentration.
- In the yellow or blue areas, the **B**-interstitials are *undersaturated* or *supersaturated*, respectively. We must expect that something new is going to happen in the supersaturated region, e.g. the precipitation of some A_xB_y compound, or a phase separation of **A** and **B**.
- On the other end of the composition axis, things would be much the same, only that now **A** is the interstitial in **B**. The equilibrium line and the melting point would be different too, of course.

The phase diagram **Pb - Sn** (familiar solder) provides a real example:



Pure lead and lead with **Sn** interstitials has a **fcc** lattice; we call this the α -phase; pure **Sn** and **Sn** with **Pb** interstitials is tetragonal, we call this the β -phase.

- In the supersaturated region something new has happened indeed, we have an *eutectic phase separation* and a mixture of α and β .
- In the high temperature regime, we have something new, too: Mixtures of liquid (**L**) and solid phases

Be that as it may (and it can be much more complicated), the essential points are

- The system always goes for the minimum free enthalpy, and this minimum could be calculated in principle following the same, albeit much more involved line of reasoning we employed for equilibrium concentrations of point defects.
- The (experimentally determined) phase diagrams are maps of the particular minimum free enthalpy configuration out of many possible arrangements for a given composition and temperature.
- Changing the temperature or the composition of a system thus takes us from one area in the phase diagram to another; the boundaries we have to cross give us an idea of what has to happen kinetically.