

Crystal defects

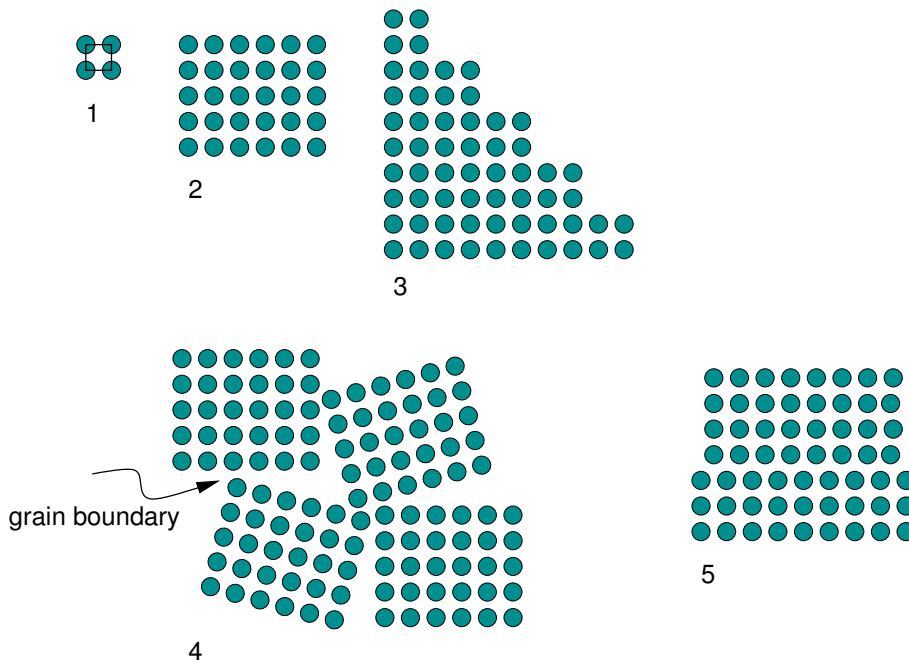
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This class closely follows the chapter 8 of Anderson, Leavay, Leavers and Rawlings

The structural hierarchy in a material

The hierarchy of structure in a polycrystalline material:

- Atoms come together in a crystal, the basic building block being the unit cell (1)
- Many unit cells make the crystal (2)
- Depending on how the unit cells are put together, the crystal's habit can change (3)
- The polycrystalline material comprises of many crystals separated by *grain boundaries* (4)
- Crystals can themselves have defects (5)



We will study the following defects (see handout)

- Vacancies and vacancy concentrations. The distribution law:

$$N_v = N \exp\left(-\frac{Q_v}{k_B T}\right)$$

where N is the total number of atomic sites, k_B is the Boltzmann constant (1.38×10^{-23} J atom⁻¹K⁻¹), Q_v is the energy to form a single vacancy, T is the temperature in K, and N_v is the fraction of vacant sites.

- Self-interstitials
- Impurity atoms (substitution and interstitials)
- Point defects — Schottky and Frenkel
- Defects and non-stoichiometry in Fe_{1-x}O
- Line defects — edge and screw dislocations and the Burgers vector
- Grain boundaries
- Planar defects — Stacking faults and twinning