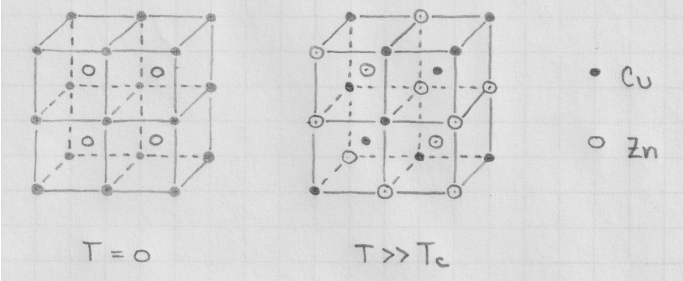
# Order-disorder transition in metallic alloys [tln95]

The binary alloy named $\beta$-brass contains copper (Cu) and zinc (Zn) in equal parts. The crystallographic structure is body-centered cubic (bcc).

The bcc lattice can be interpreted as two interpenetrating simple cubic (sc) sublattices 1 and 2.

In the ground state, i.e. at $T = 0$, the Cu atoms occupy one sublattice and the Zn atoms the other. At high temperature, the average Cu and Zn occupancies of each lattice site on both sublattices are the same:

$$\langle n_{\mathrm{Cu}}^{(1)} \rangle = \langle n_{\mathrm{Cu}}^{(2)} \rangle = \langle n_{\mathrm{Zn}}^{(1)} \rangle = \langle n_{\mathrm{Zn}}^{(2)} \rangle = \frac{1}{2}.$$




Thermal fluctuations facilitate hopping of atoms between nearest-neighbor sites in groups without affecting the lattice structure.

A continuous order-disorder phase transition is observed to take place at $T_{\mathrm{c}} = 733\mathrm{K}$. The order parameter,

$$m \doteq \langle n_{\mathrm{Cu}}^{(1)} \rangle - \langle n_{\mathrm{Cu}}^{(2)} \rangle = \langle n_{\mathrm{Zn}}^{(2)} \rangle - \langle n_{\mathrm{Zn}}^{(1)} \rangle,$$

is identically zero at $T > T_{\mathrm{c}}$ and grows continuously out of a cusp singularity from zero toward unity as $T$ is lowered from $T_{\mathrm{c}}$ toward zero.

The (ordered) macrostate at $T < T_{\mathrm{c}}$ has a lower translational symmetry than the (disordered) macrostate at $T > T_{\mathrm{c}}$. The symmetry of the disordered state is broken by the ordered state.

A simple model Hamiltonian for this transition distinguishes three distinct interaction energies, $E_{\mathrm{CuCu}}$, $E_{\mathrm{ZnZn}}$, and $E_{\mathrm{CuZn}}$, between nearest-neighbor atoms on the bcc lattice:

$$\mathcal{H} = \sum_{\langle ij \rangle} \Big[ E_{\mathrm{CuCu}} n_i^{(\mathrm{Cu})} n_j^{(\mathrm{Cu})} + E_{\mathrm{ZnZn}} n_i^{(\mathrm{Zn})} n_j^{(\mathrm{Zn})} + E_{\mathrm{CuZn}} \big( n_i^{(\mathrm{Cu})} n_j^{(\mathrm{Zn})} + n_i^{(\mathrm{Zn})} n_j^{(\mathrm{Cu})} \big) \Big],$$

where the sum $\langle ij \rangle$ is over all nearest-neighbor pairs of the bcc lattice.

The equivalent Ising model emerges via transcription from lattice occupation numbers $n_i^{(\mathrm{Cu})} = 1 - n_i^{(\mathrm{Zn})} = 0, 1$ to Ising spins $\sigma_i = \pm 1$:

$$n_i^{(\mathrm{Cu})} = \frac{1}{2}(1 + \sigma_i), \quad n_i^{(\mathrm{Zn})} = \frac{1}{2}(1 - \sigma_i).$$

$$\Rightarrow \; \mathcal{H} = \frac{1}{8} z N \Big[ E_{\mathrm{CuCu}} + E_{\mathrm{ZnZn}} + 2E_{\mathrm{CuZn}} \Big] + \underbrace{\frac{1}{4} z \Big[ E_{\mathrm{CuCu}} - E_{\mathrm{ZnZn}} \Big]}_{H} \underbrace{\sum_i \sigma_i}_{0}$$

$$+ \underbrace{\frac{1}{4} \Big[ E_{\mathrm{CuCu}} + E_{\mathrm{ZnZn}} - 2E_{\mathrm{CuZn}} \Big]}_{J} \sum_{\langle ij \rangle} \sigma_i \sigma_j .$$

- The first term is a constant: the reference energy $E_0$.
- The second term vanishes when the numbers of Cu and Zn atoms are equal (as assumed).
- If the alloy contains different numbers of Cu and Zn atoms, the Ising model must include the coupling to an external field $H$.
- The coefficient of the last term becomes the coupling constant $J$ of the Ising model. In $\beta$-brass $J > 0$ is realized.

$$\mathcal{H} = E_0 + H \sum_i \sigma_i + J \sum_{\langle ij \rangle} \sigma_i \sigma_j .$$