Karlsruhe Institute of Technology

Institute for Applied Materials

Plasticity

Lecture for “Mechanical Engineering” and “Materials Science and Engineering”
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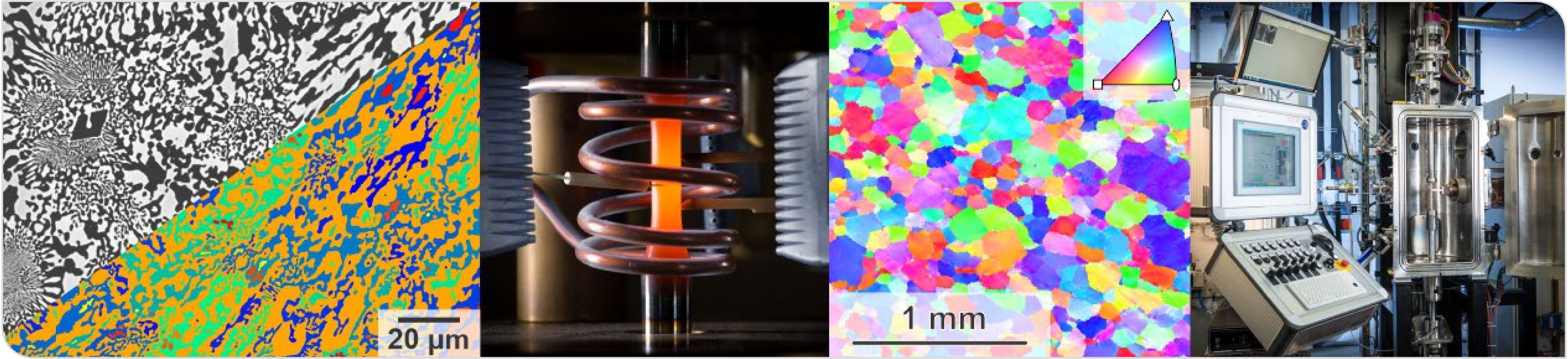
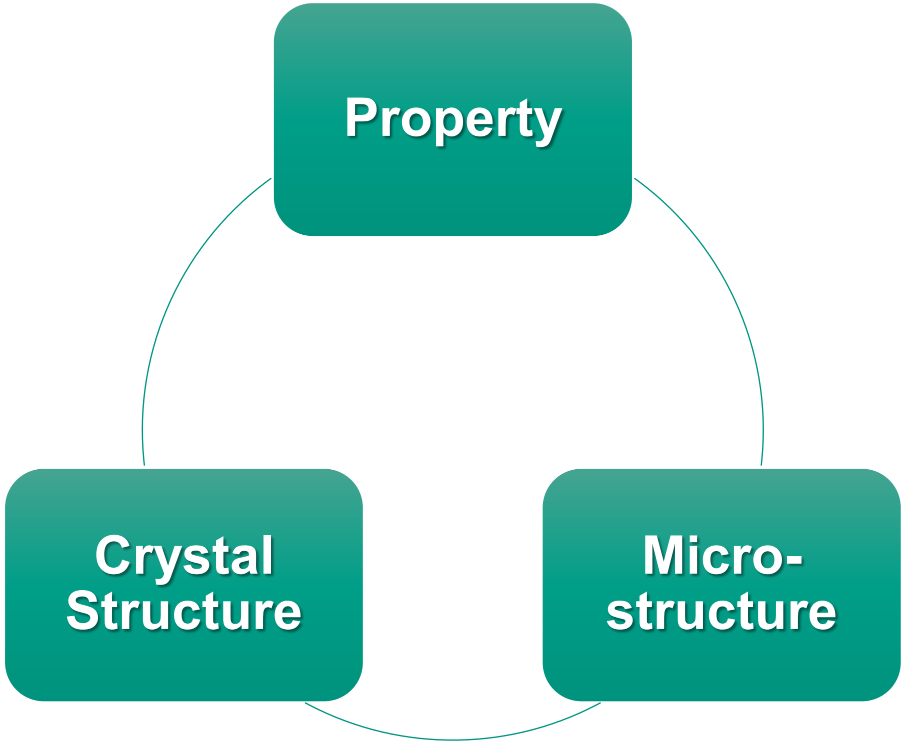


Topics

- Classification of Defects
- Some Defects
  - Vacancies
  - Solutes & Complex Point Defects
  - Line Defects
  - Grain Boundaries
    - Tilt and Twist Boundaries
    - Low Angle and High Angle Grain Boundaries
    - Twin Boundaries
    - Coincidence Site Lattice and Displacement Shift Complete
  - Stacking Faults

Structure-Microstructure-Property Relationship



All features determined by the thermodynamic equilibrium state

All features that are not determined by thermodynamic equilibrium state

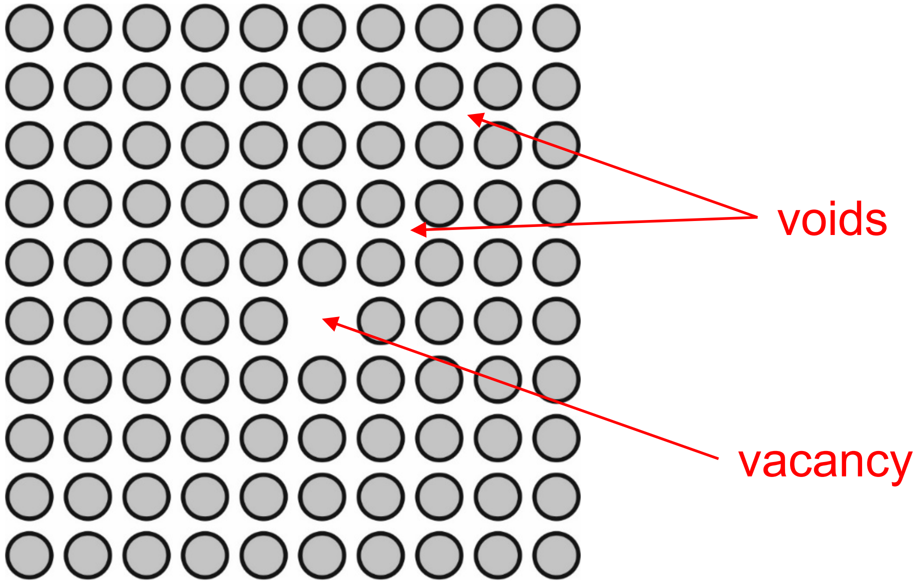
Of course, **most features discussed in this class are related to deviations (defects) from thermodynamic ground state**! Nevertheless, the description of deviations needs a **proper understanding of the ideal state**. Hence, crystallography provides the basis for any defect classification.

Defect Classification

- Most of the important engineering properties of metals and intermetallics are determined by crystal defects. We usually classify them according to their dimensionality:
  - Point defects, 0D:
    - vacancies
    - interstitial and substitutional atoms
    - complex point defects
  - Line defects, 1D:
    - dislocations (Ch. 4)
    - disclinations
  - Planar defects, 2D:
    - grain boundaries
    - phase boundaries
    - stacking faults
    - surfaces
  - Bulk defects, 3D:
    - precipitates, dispersoids
    - cracks
    - pores
- In the following, only aspects are repeated which will become important during this class. In certain cases, more details are provided in the respective lectures on the defects.

Vacancies

- Vacancies are vacant lattice sites. In contrast to voids, vacancies have to form under expense of energy. Voids are intrinsic part of the crystal structure.



Vacancies

- Due to the entropy contribution and comparably low formation enthalpy, vacancies are present in thermodynamic equilibrium. The Gibb's free energy change due to N_V vacancies in an crystal of N atoms is:

$$\Delta G_\mathrm{V} = \Delta H_\mathrm{V} - T \cdot \Delta S_\mathrm{V} = N_\mathrm{V} \cdot \Delta H_\mathrm{V}^\mathrm{F} - T \cdot \left(N_\mathrm{V} \cdot \Delta S_\mathrm{V}^\mathrm{P} + \Delta S_\mathrm{V}^\mathrm{mix}\right)$$

- $\Delta H_\mathrm{V}^\mathrm{F}$ denotes the enthalpy of formation of vacancies, $\Delta S_\mathrm{V}^\mathrm{P}$ is the change in vibration states due to the vacancies and $\Delta S_\mathrm{V}^\mathrm{mix}$ is the configurational entropy change:

$$\Delta S_\mathrm{V}^\mathrm{mix} = S_\mathrm{faulted} - S_\mathrm{perfect} = k_\mathrm{B} \cdot \ln \frac{N!}{N_\mathrm{V}! \cdot (N - N_\mathrm{V})!} - k_\mathrm{B} \cdot \ln 1$$

$$= k_\mathrm{B} \cdot (\ln N! - \ln N_V! - \ln(N - N_\mathrm{V})!)$$

- Using Stirling's approximation for factorials:

$$\Delta S_\mathrm{V}^\mathrm{mix} \approx k_\mathrm{B} \cdot \left(N \ln N - N - N_\mathrm{V} \ln N_\mathrm{V} + N_\mathrm{V} - (N - N_\mathrm{V}) \ln(N - N_\mathrm{V}) + (N - N_\mathrm{V})\right)$$

$$= k_\mathrm{B} \cdot (N \ln N - N_\mathrm{V} \ln N_\mathrm{V} - (N - N_\mathrm{V}) \ln(N - N_\mathrm{V}))$$

Vacancies

- Thermodynamic equilibrium with the equilibrium concentration x_V^0 is then:

$$\left.\frac{\mathrm{d}\,\Delta G_\mathrm{V}}{\mathrm{d}N_\mathrm{V}}\right|_{N_\mathrm{V}^0} = \Delta H_\mathrm{V}^\mathrm{F} - T \cdot \Delta S_\mathrm{V}^\mathrm{P} - T \cdot \frac{\mathrm{d}\,\Delta S_\mathrm{V}^\mathrm{mix}}{\mathrm{d}N_\mathrm{V}} = 0$$

$$\Delta H_\mathrm{V}^\mathrm{F} - T \cdot \Delta S_\mathrm{V}^\mathrm{P} - T \cdot \frac{\mathrm{d}\,\Delta S_\mathrm{V}^\mathrm{mix}}{\mathrm{d}N_\mathrm{V}} = 0$$

$$\Delta H_\mathrm{V}^\mathrm{F} - T \cdot \Delta S_\mathrm{V}^\mathrm{P} + T \cdot \left(k_\mathrm{B} \cdot \ln \frac{N_\mathrm{V}^0}{N - N_\mathrm{V}^0}\right) \approx \Delta H_\mathrm{V}^\mathrm{F} - T \cdot \Delta S_\mathrm{V}^\mathrm{P} + T \cdot k_\mathrm{B} \cdot \ln \frac{N_\mathrm{V}^0}{N} = 0$$

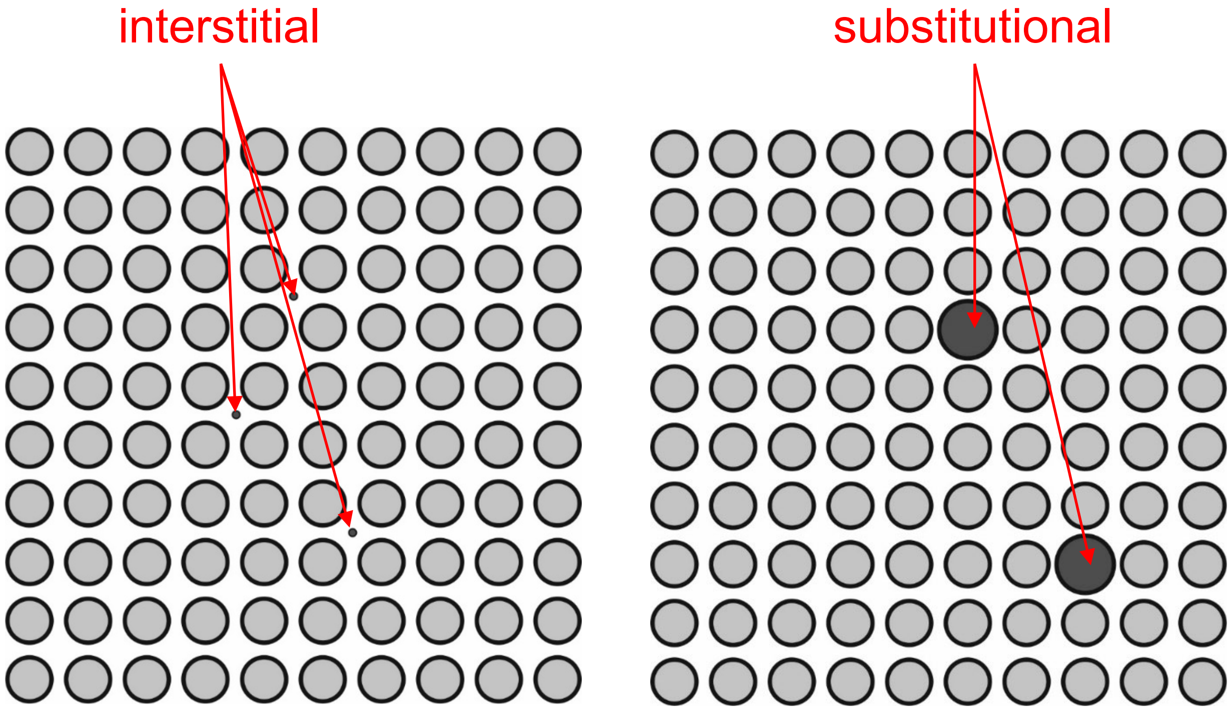
$$x_\mathrm{V}^0 = \frac{N_\mathrm{V}^0}{N} = \exp\left(\frac{T \cdot \Delta S_\mathrm{V}^\mathrm{P} - \Delta H_\mathrm{V}^\mathrm{F}}{T \cdot k_\mathrm{B}}\right) = \exp\left(\frac{\Delta S_\mathrm{V}^\mathrm{P}}{k_\mathrm{B}}\right) \cdot \exp\left(-\frac{\Delta H_\mathrm{V}^\mathrm{F}}{T \cdot k_\mathrm{B}}\right)$$

$$x_\mathrm{V}^0 \propto \exp\left(-\frac{\Delta H_\mathrm{V}^\mathrm{F}}{T \cdot k_\mathrm{B}}\right)$$

- Equ. vacancy density at about solidus temperature is in the order of 10^{-4}.

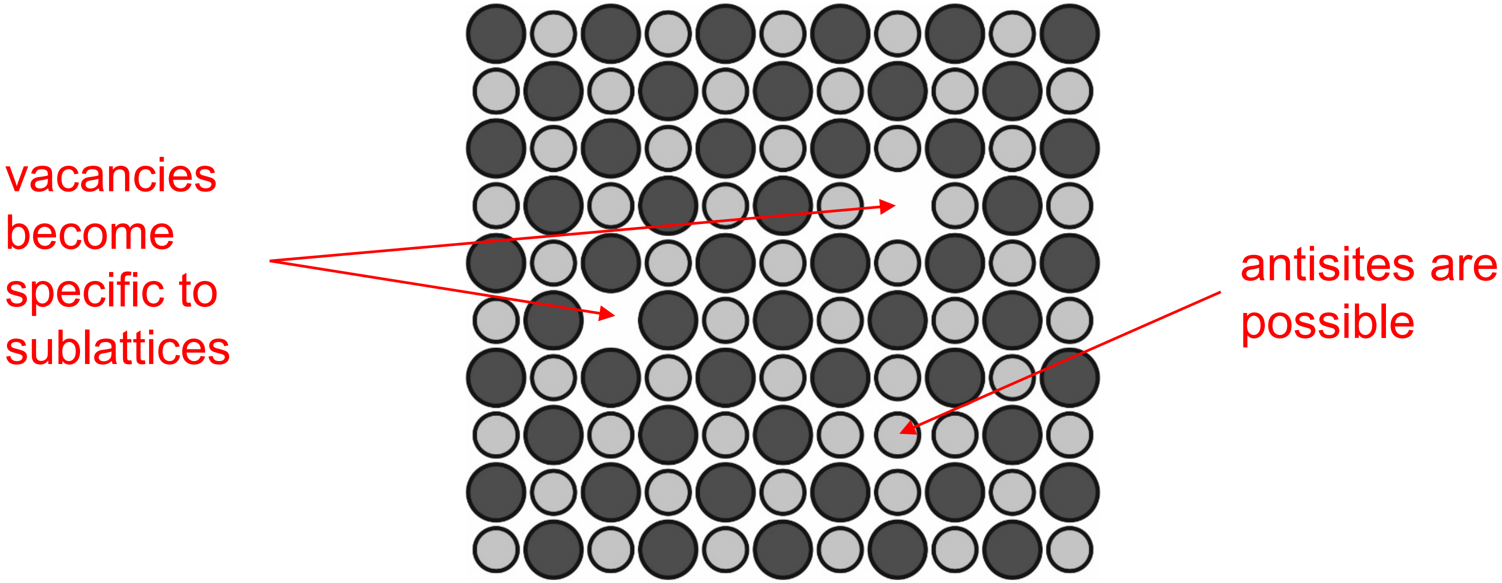
Solutes

- Solutes can substitute atoms on lattice sites or can be dissolved in voids depending on their properties. Depending on the symmetry of the position, strain fields can be hydrostatic or with deviatoric contributions.



Complex Point Defects

- In intermetallic compounds, more complex forms of point defects or combinations of point defects are possible due to the presence of order.



vacancies become specific to sublattices

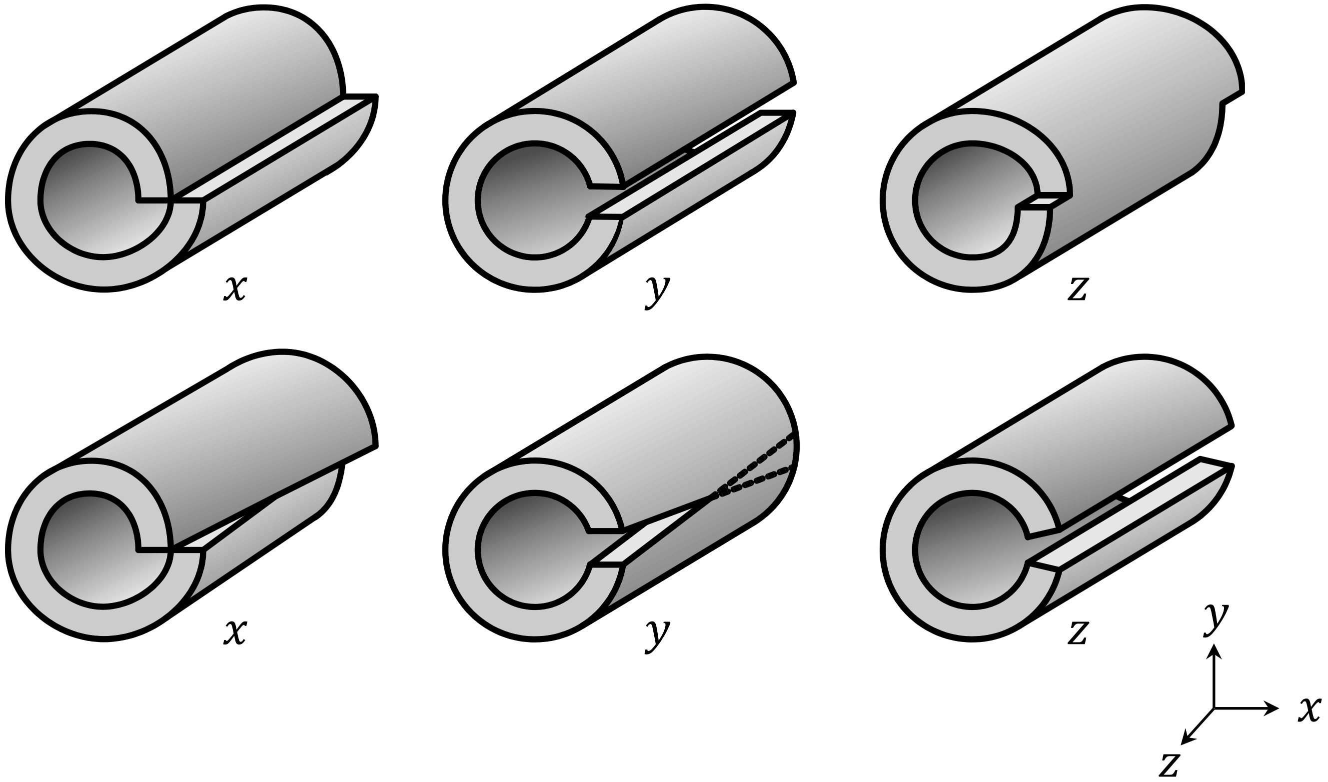
antisites are possible

Line Defects

- In general, multiple types of line defects are possible. Dislocations of mixed character between edge and screw dislocation are of course the most important for plasticity. Therefore, Ch. 4 will intensively deal with them:

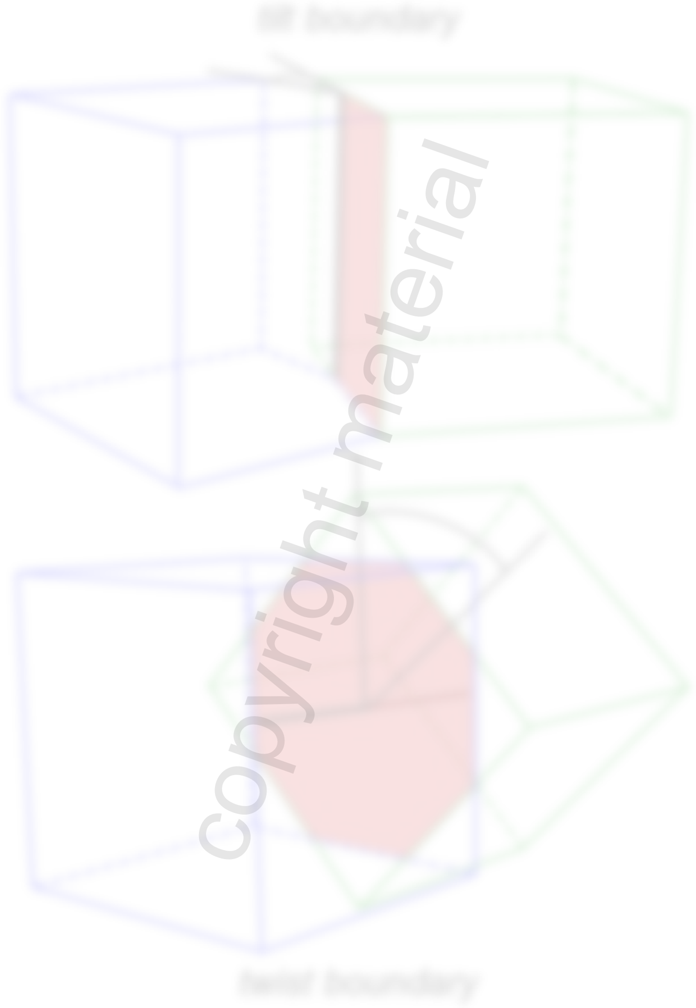
Dislocation
(The crystal is cut along a line, displaced by a certain magnitude in a certain direction, and finally rejoined.)

Disclination
(The crystal is cut along a line, rotated of a certain magnitude about a certain direction, and finally rejoined.)



Grain Boundaries

- **Grain boundaries** are 2D defects that **separate crystal of the same phase but different orientation**. We will distinguish **low angle grain boundaries (LAGB)**, **high angle grain boundaries (HAGB)** and **twin boundaries**.
- **Eight independent parameters are needed** to describe grain boundaries:
  - three angles for the rotation of the systems
  - three components for the translation vector of the systems
  - two components for the description of the plane between the crystals
- **Tilt and twist boundaries are easy cases** which reduce the number of parameters by assuming rotation axes perpendicular or within the grain boundary.

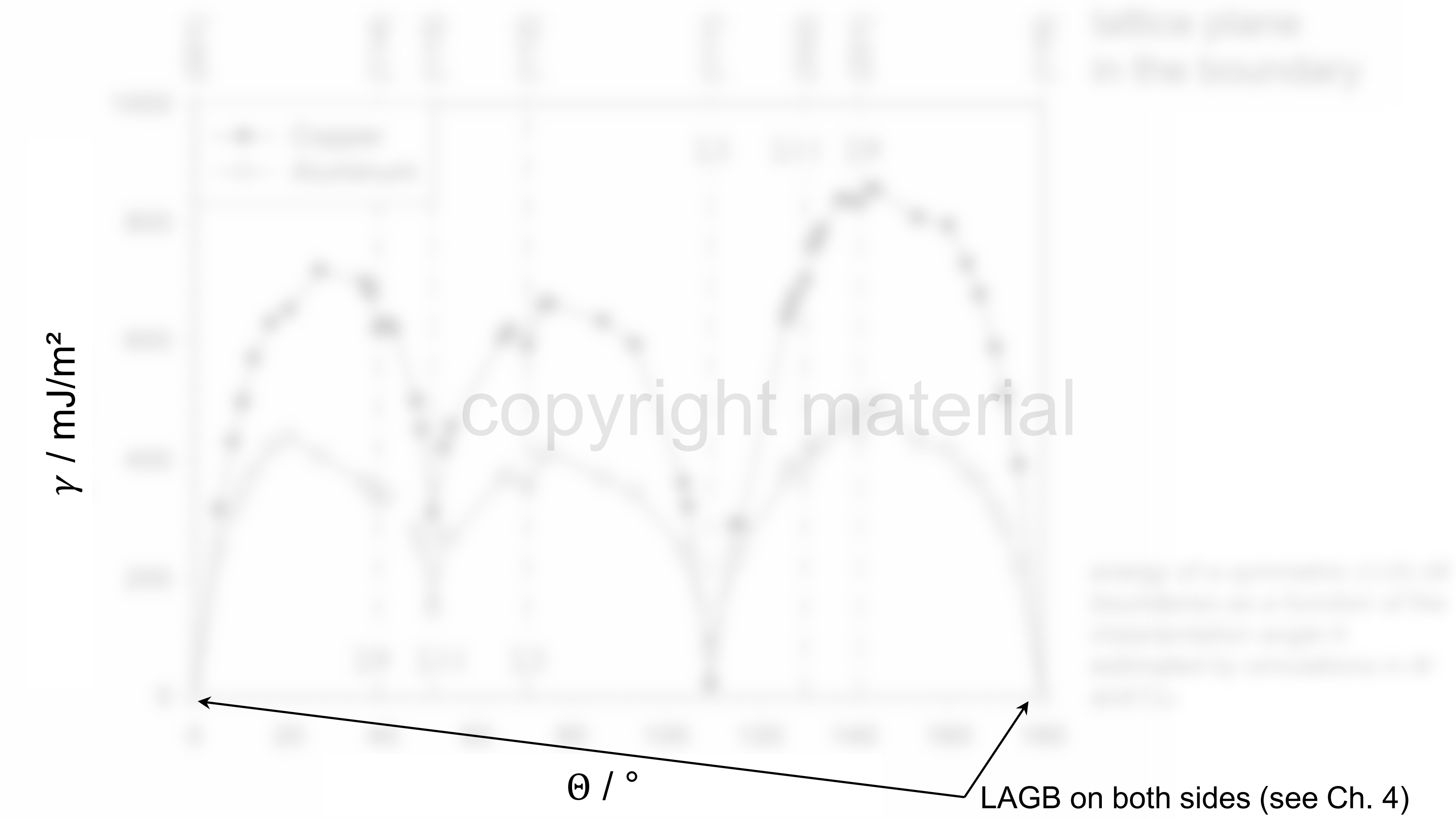


https://en.wikipedia.org/wiki/Grain_boundary#/media/File:TiltAndTwistBoundaries_remade.svg

Grain Boundaries

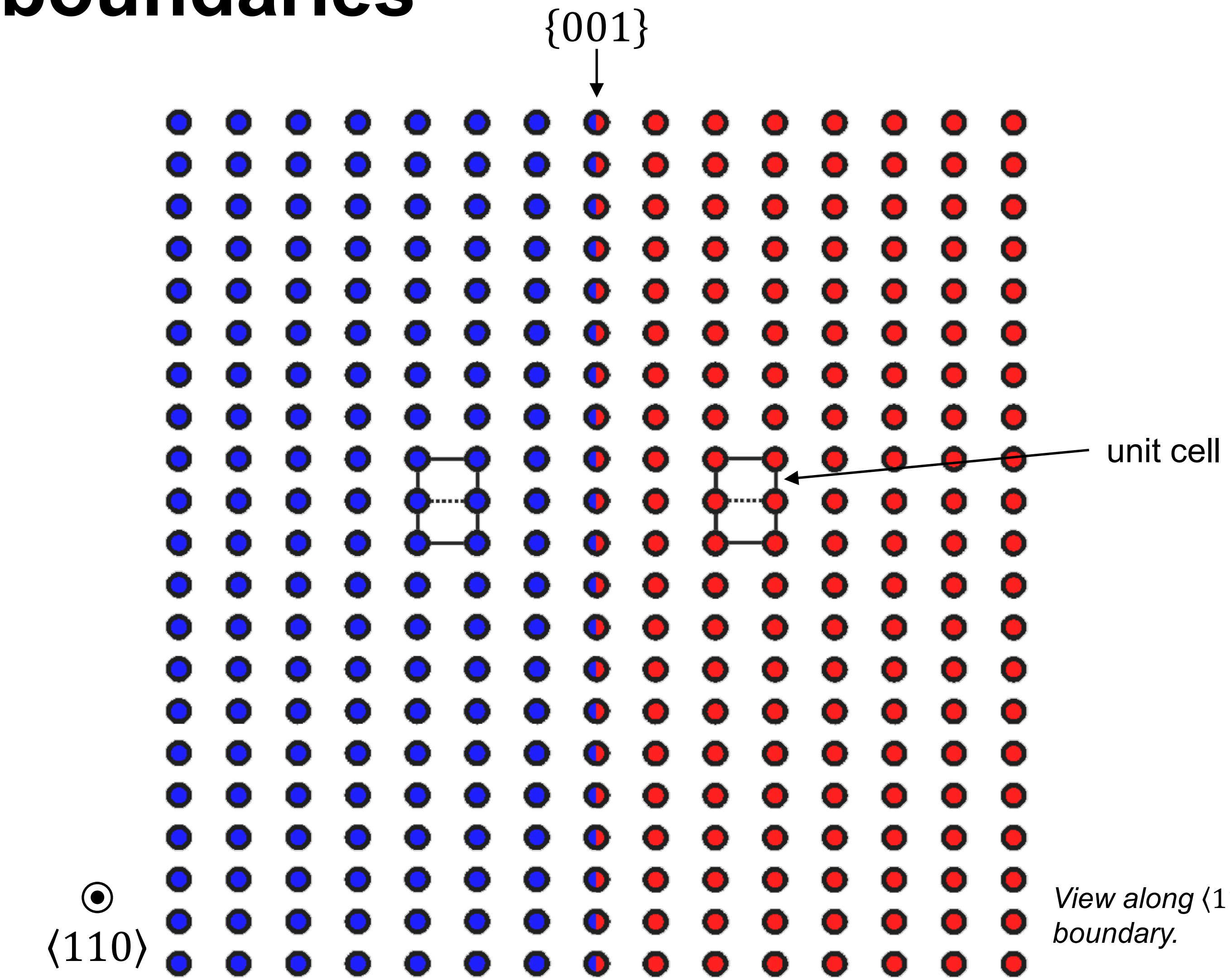
- There are two possible ways to **distinguish LAGB and HAGB**, namely **by misorientation** or **by mobility**:
  - LAGB can be described by metastable arrangements of dislocations. The upper limit of that description is about $10 \ldots 15°$. The cut-off corresponds to a geometrical interpretation of the defect. We will discuss this model in Ch. 4.
  - The movement of LAGB needs a cooperative movement of all dislocation mentioned above. Hence, LAGB considered as immobile in comparison to HAGB. The transition in mobility is at about $12°$ in misorientation.

Grain Boundaries



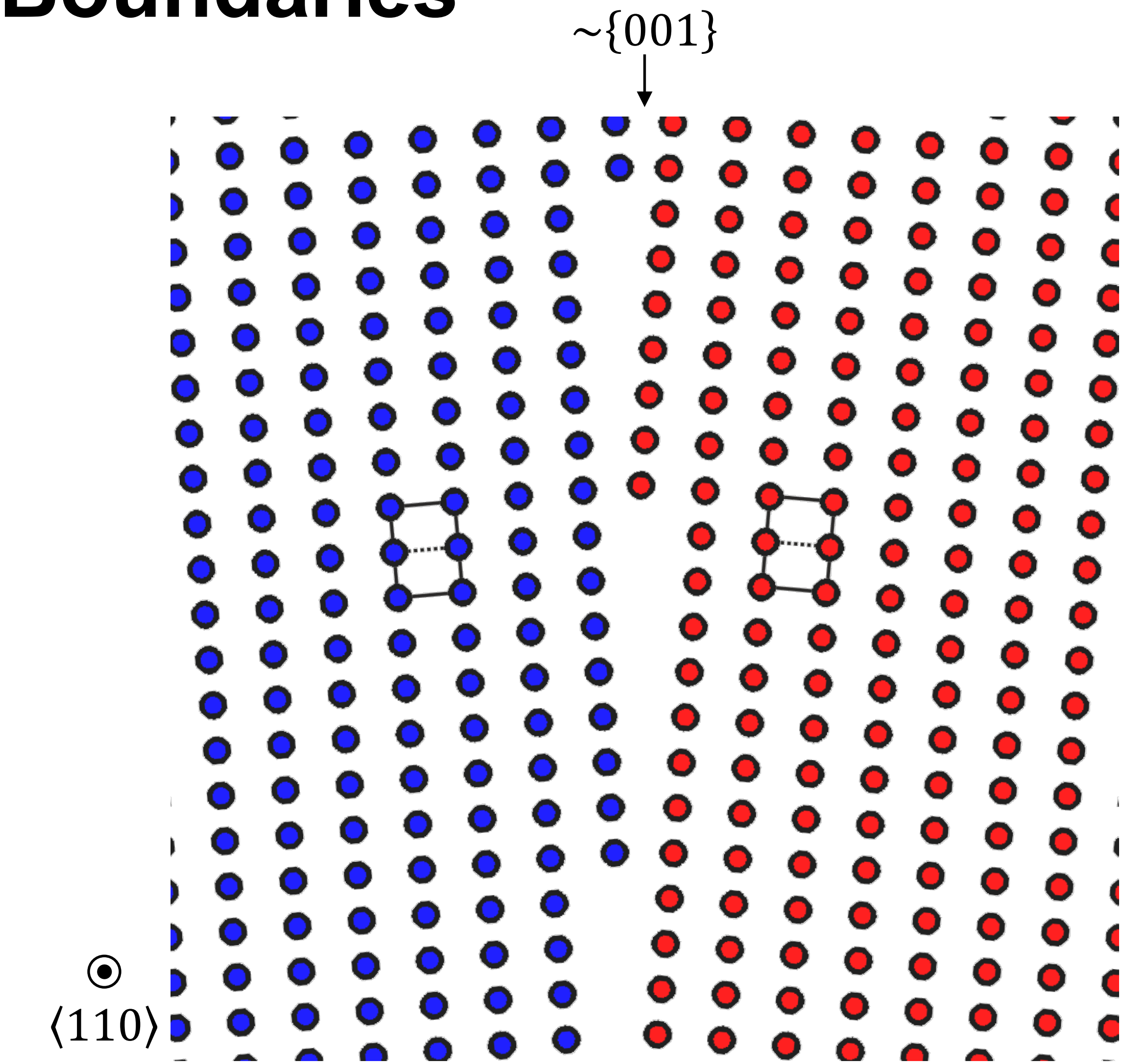
M.A. Tschopp, D.E. Spearot, D.L. McDowell: "Influence of Grain Boundary Structure on Dislocation Nucleation in FCC Metals" in "Dislocations in Solids“, J.P. Hirth (ed.), Vol. 14, Elsevier, Amsterdam (2008) pp. 43-140

Grain boundaries



View along ⟨110⟩ *in fcc A1. No boundary.*

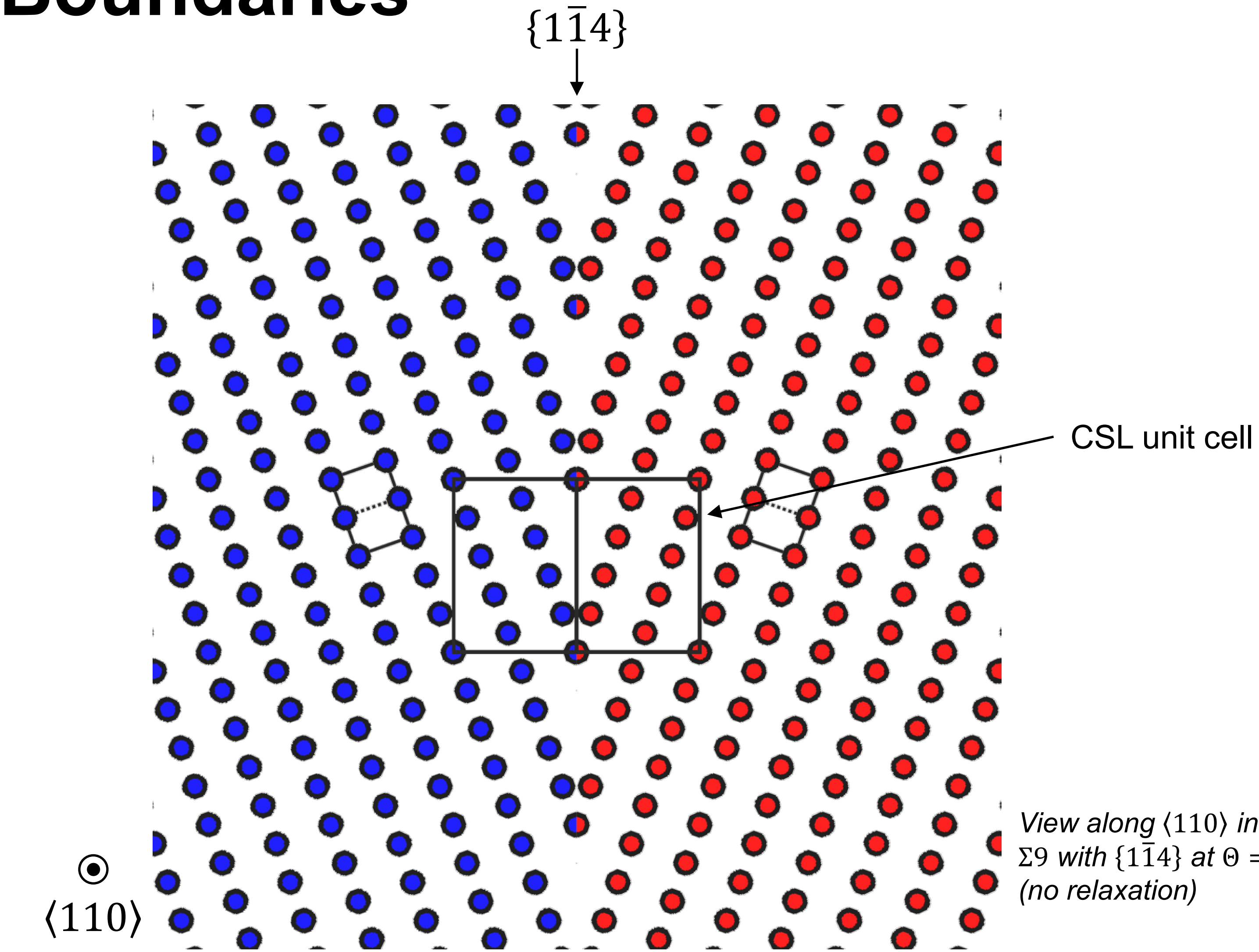
Grain Boundaries



(see Ch. 4)

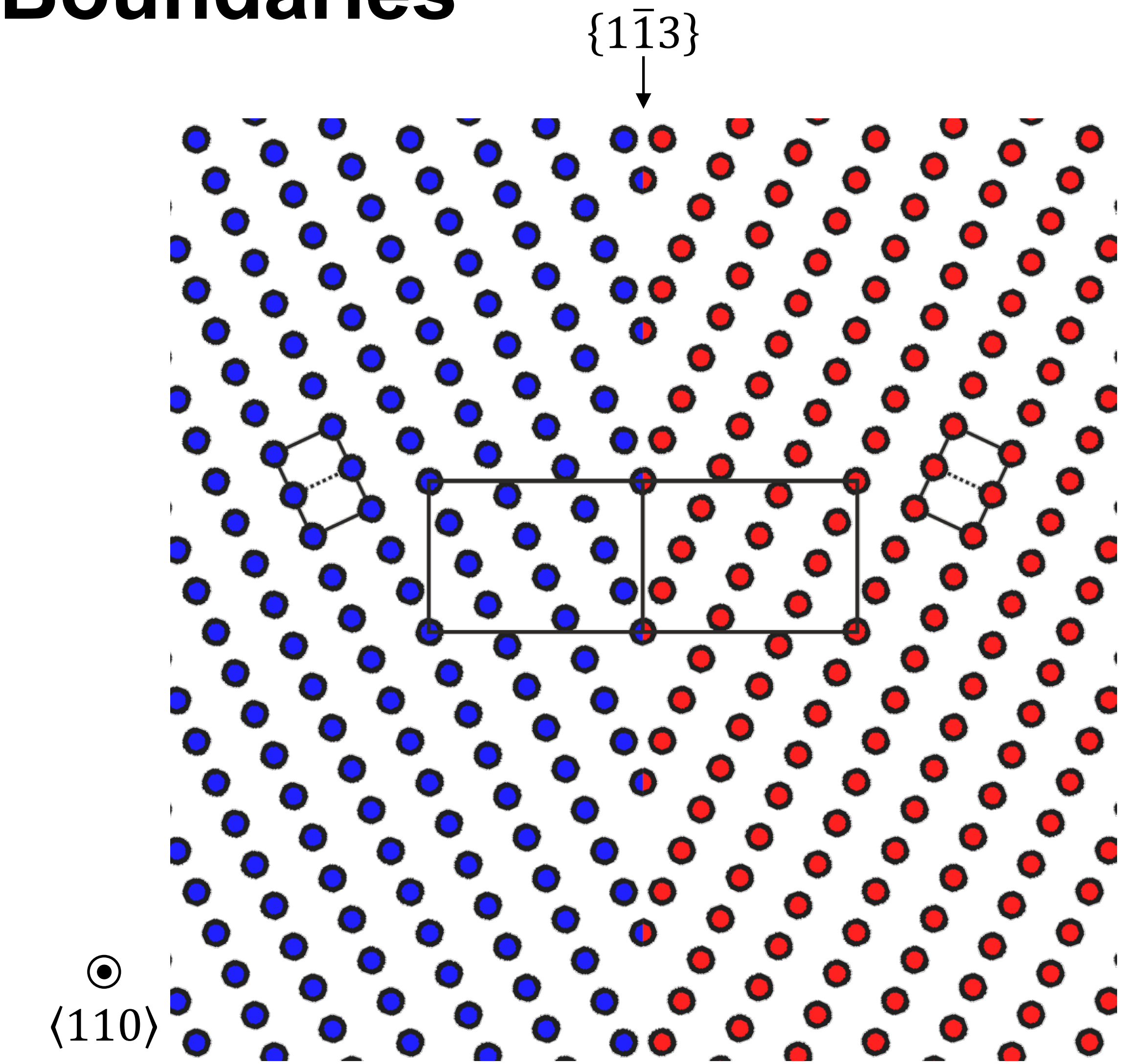
View along $\langle 110 \rangle$ in fcc A1: low angle boundary built from dislocations with $\Theta \approx 10°$.
(no relaxation)

Grain Boundaries



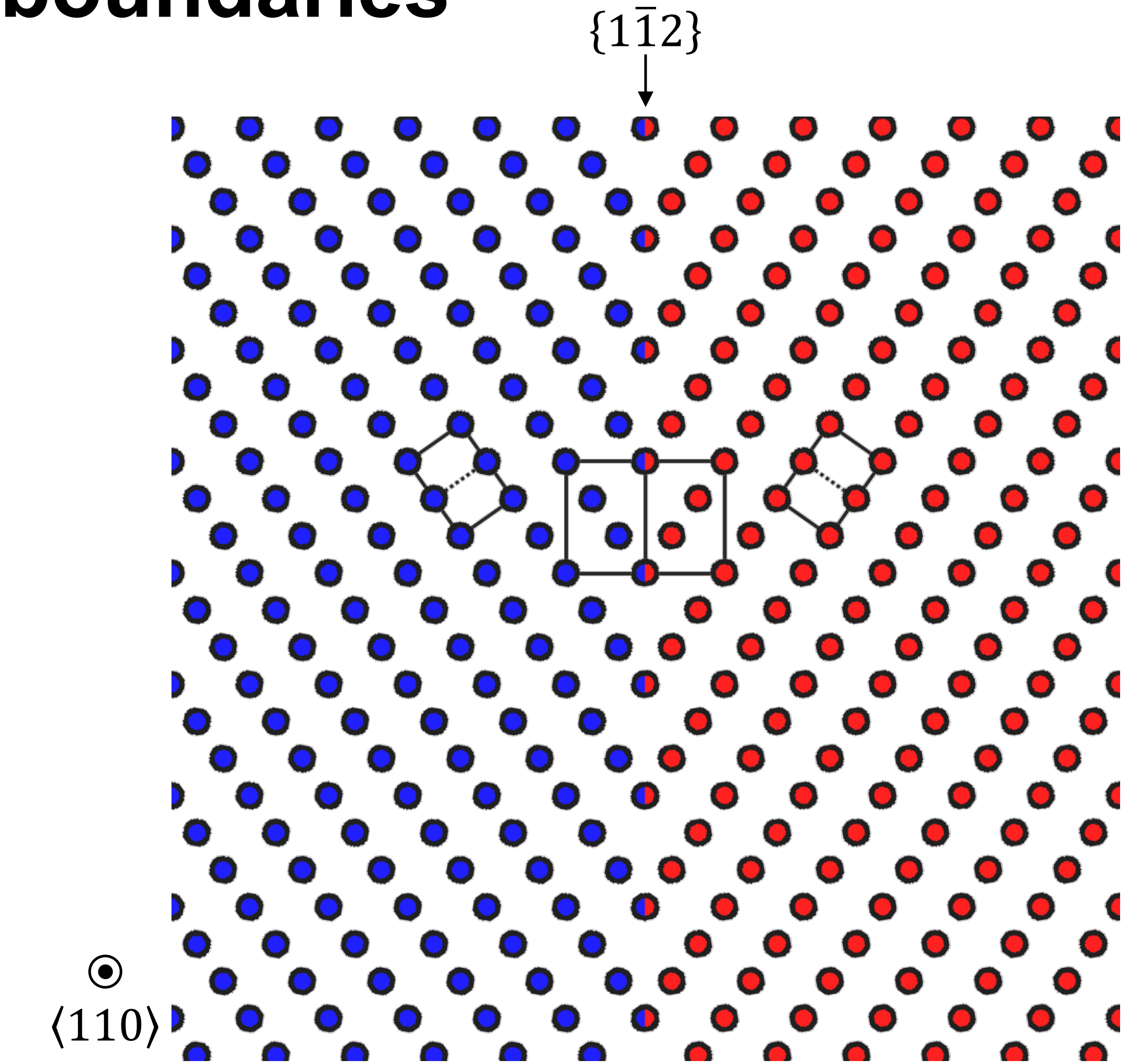
View along $\langle 110 \rangle$ *in fcc A1:*
$\Sigma 9$ *with* $\{1\bar{1}4\}$ *at* $\Theta = 38.9°$.
(no relaxation)

Grain Boundaries



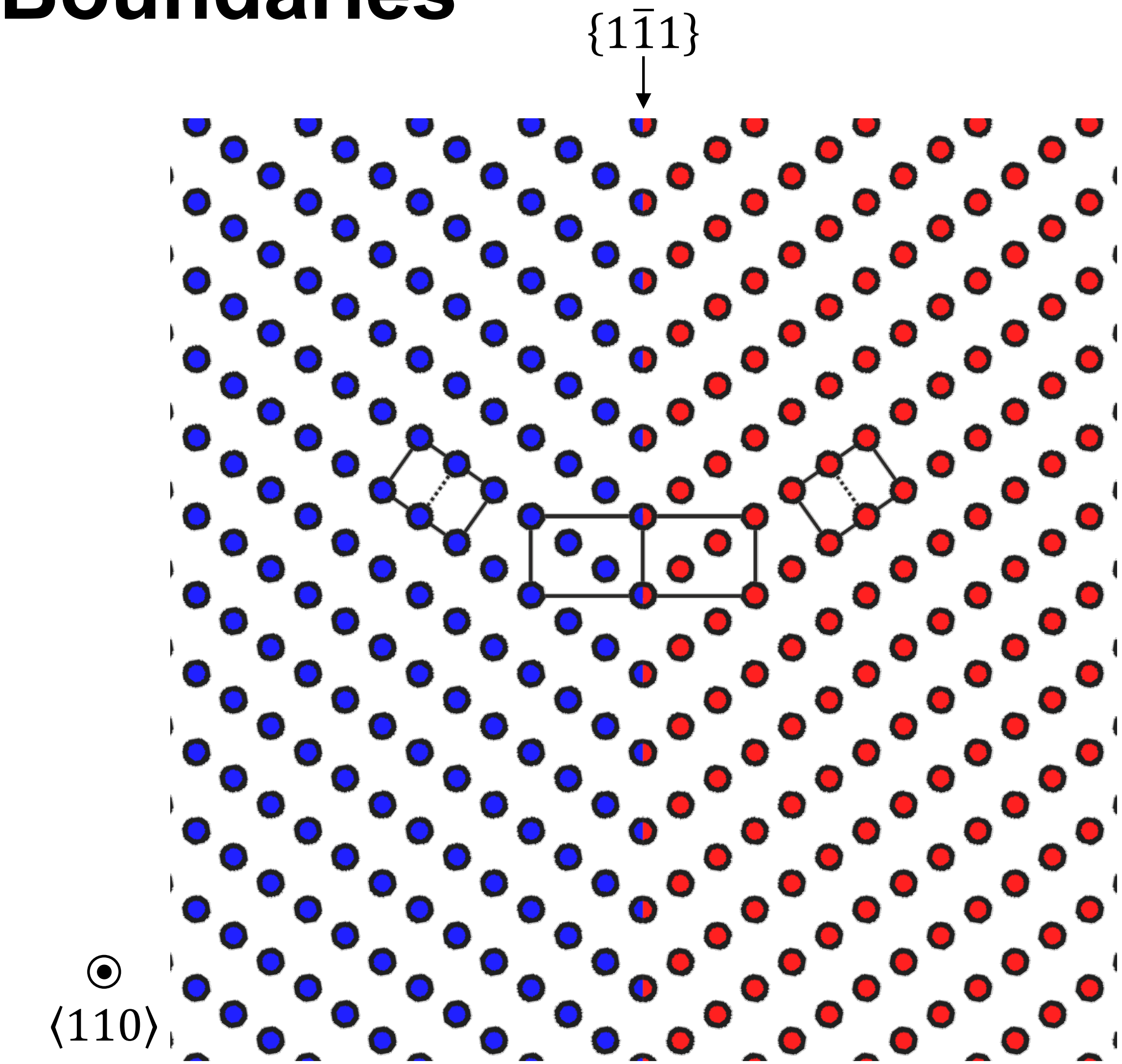
View along $\langle 110 \rangle$ *in fcc A1:*
$\Sigma 11$ *with* $\{1\bar{1}3\}$ *at* $\Theta = 50.5°$*.*
(no relaxation)

Grain boundaries



View along $\langle 110 \rangle$ *in fcc A1:*
$\Sigma 3$ *with* $\{1\bar{1}2\}$ *at* $\Theta = 70.5°$.
(no relaxation)

Grain Boundaries



View along $\langle 110 \rangle$ *in fcc A1:*
$\Sigma 3$ *with* $\{1\bar{1}1\}$ *at* $\Theta = 109.5°$.
(no relaxation)

Grain Boundaries

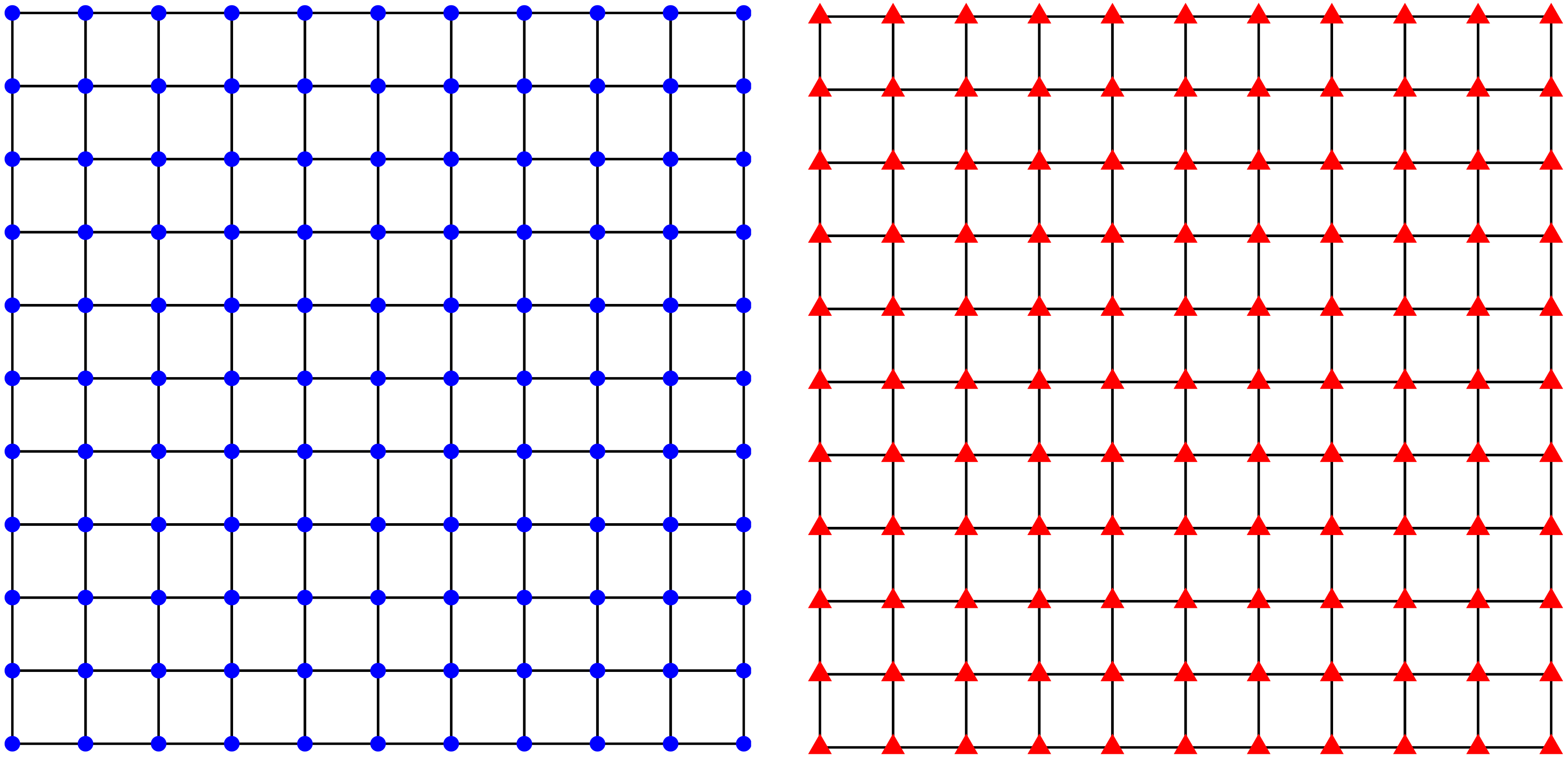
- Twin boundaries are **special boundaries when the orientation relationship of the two crystals** can be described **by a distinct symmetry operation**; the symmetry operation must not be an elements of the crystal structure in order to obtain an orientation difference.
- Depending on the symmetry operation different types of twin boundaries can be distinguished:
  - translation (in metals these are essentially stacking faults; in intermetallic compounds these can be stacking faults, antiphase boundaries or complex faults)
  - inversion
  - **rotation**
  - **mirroring**
- The latter two will be of importance when discussing deformation twinning later in the class because they come along with a shear deformation of the crystal.

Grain Boundaries

- As indicated by the energy vs. misorientation plot, there are special boundaries at intermediate angles, the energy of which is low.
- In these cases, periodic structures across the boundaries are obtained and that lead to a reduction in energy.
- There are different approaches to describe these periodic structures:
  - There is a lattice, each lattice point of which is occupied by an atom (coincidence site lattice, CSL).
  - There is the coarsest lattice, that describes all atoms on both sides of the boundary (displacement shift complete, DSC).
- Hence, the unit cell of the CSL is greater than the unit cell of the crystals whereas the DSC unit cell is smaller.

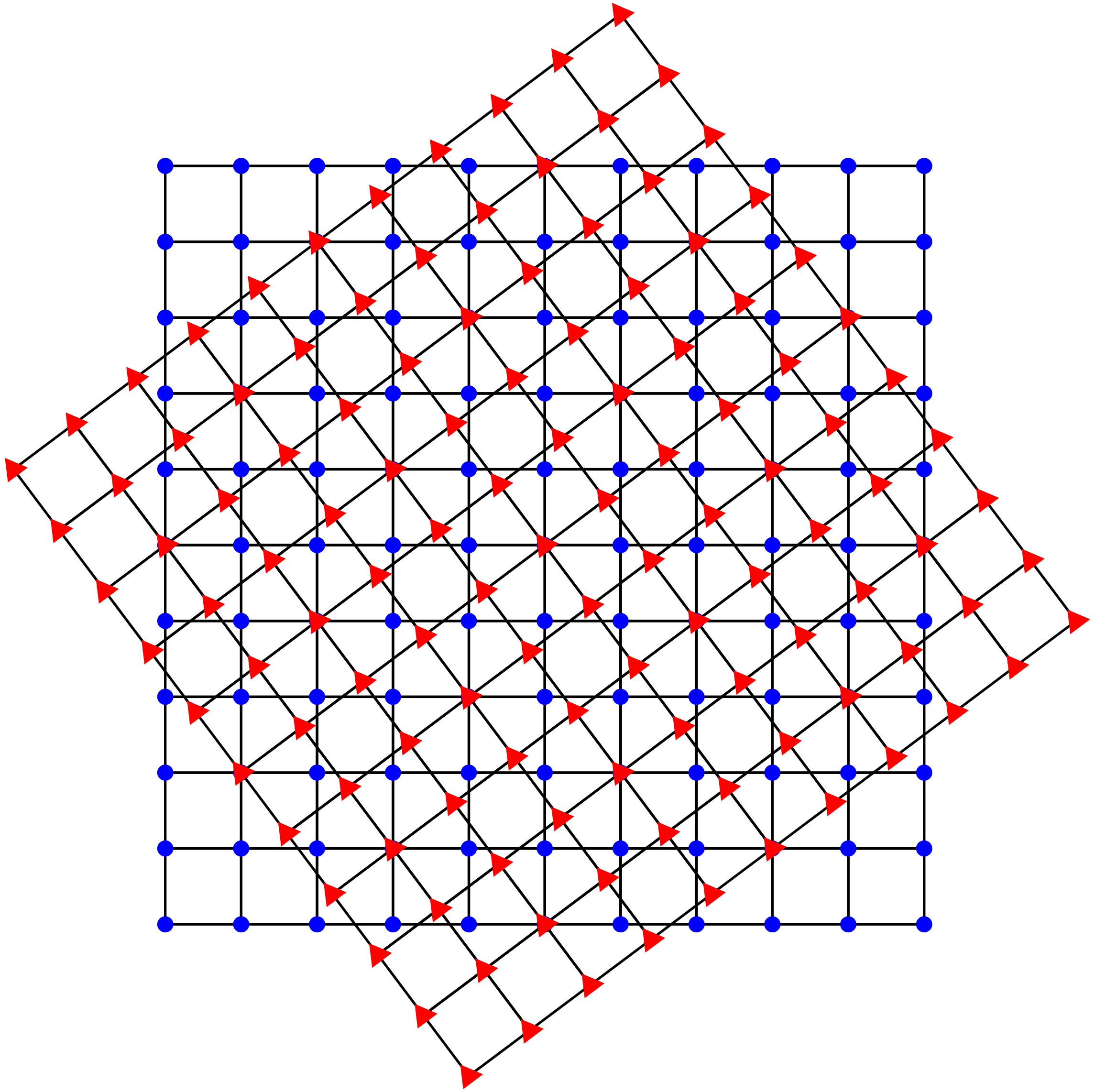
Site Lattices, Try It Yourself

Two 2D cubic „grains“.



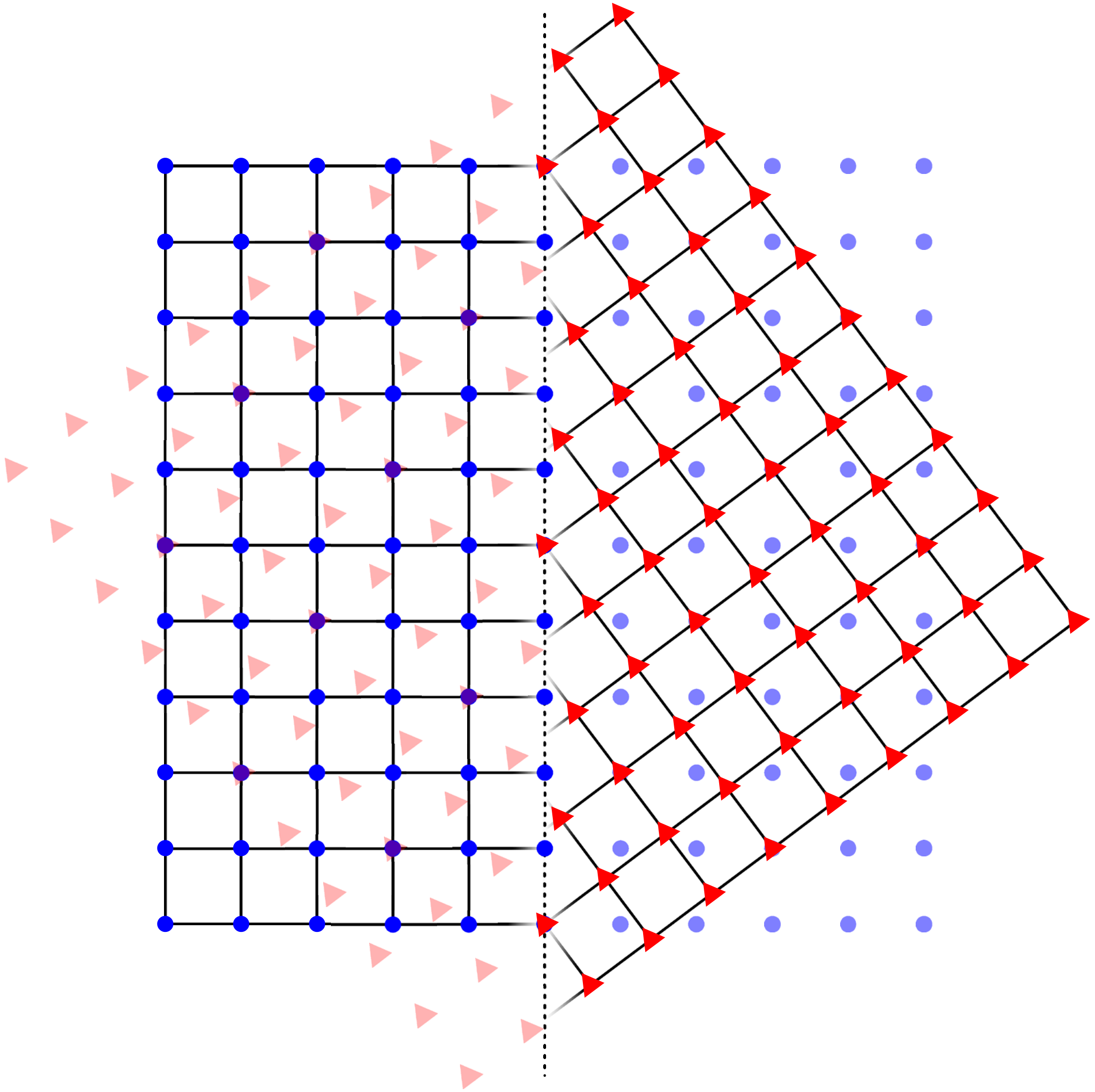
Print it on transparent sheet.

Site Lattices



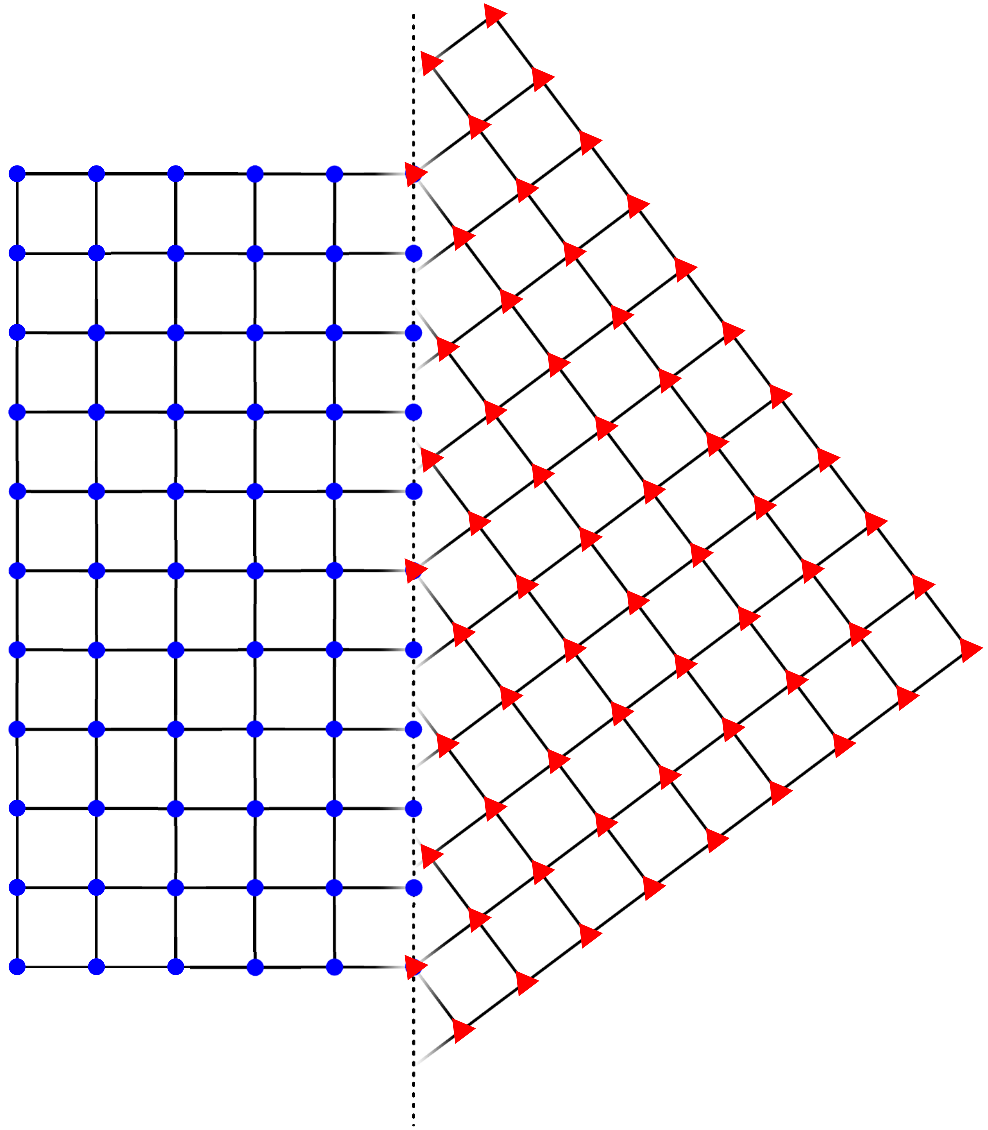
CSL with $\Sigma5$:
$36.87°$ about $[001]$

Site Lattices



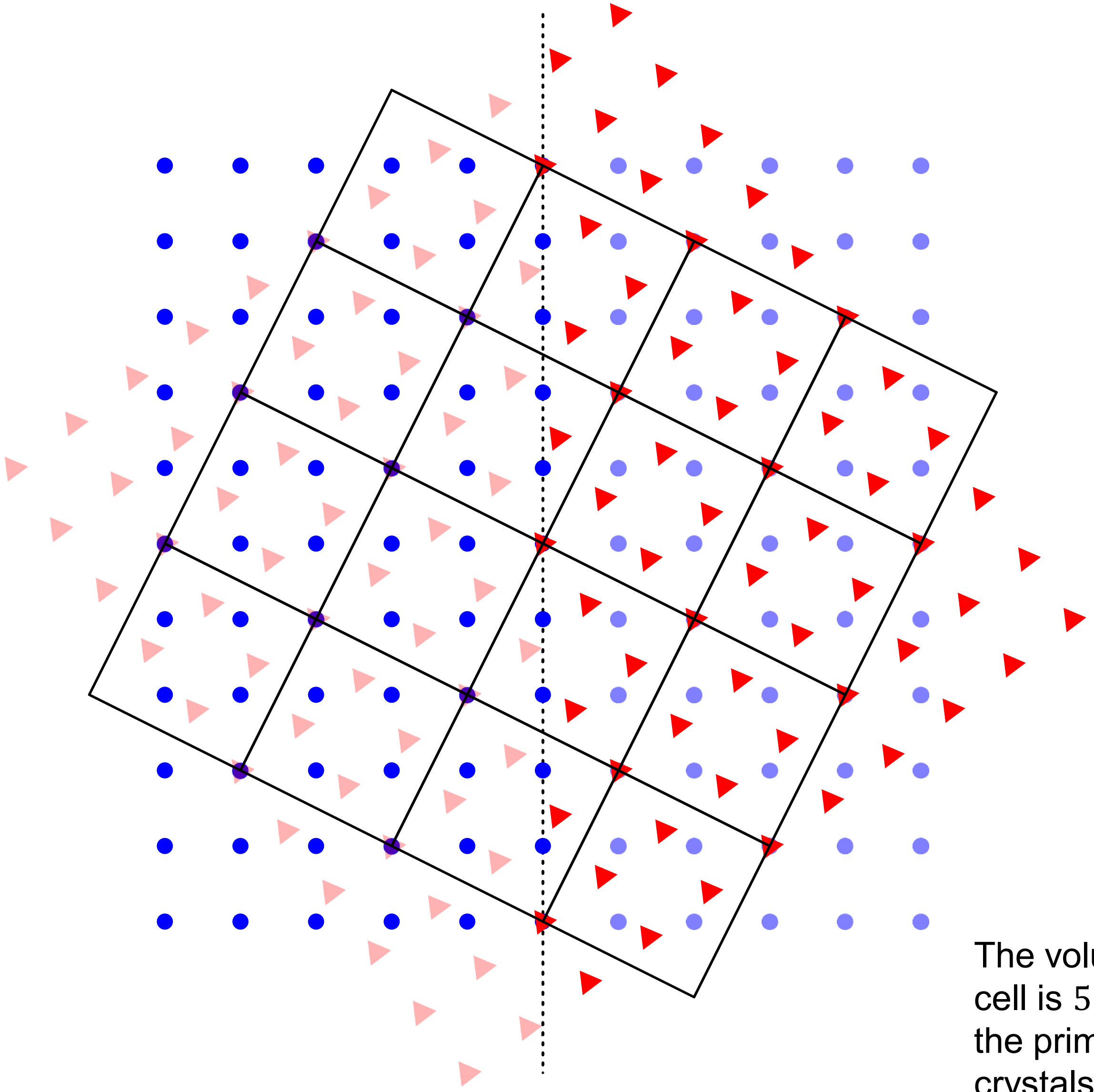
CSL with $\Sigma 5$:
$36.87°$ about $[001]$

Site Lattices



CSL with $\Sigma 5$:
$36.87°$ about $[001]$

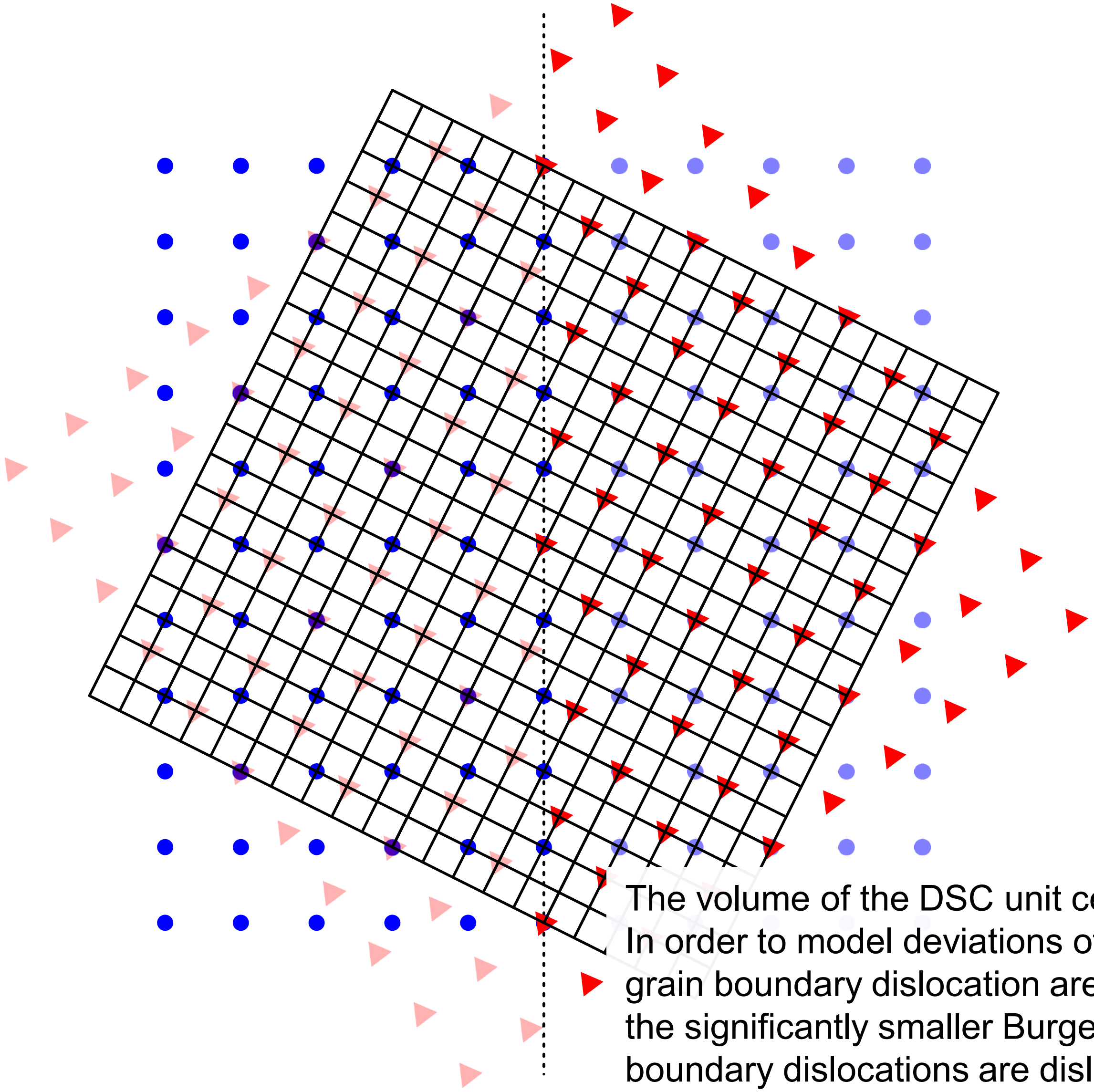
Site Lattices



CSL with $\Sigma 5$:
$36.87°$ about $[001]$

The volume of the CSL unit cell is 5 times the volume of the primitive cells of the crystals.

Site Lattices

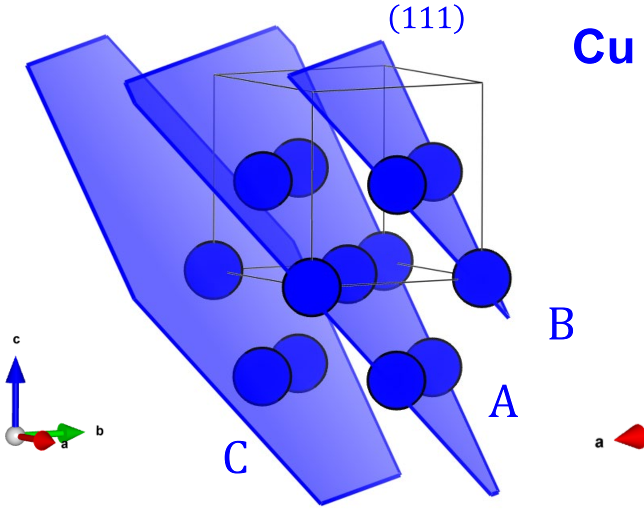


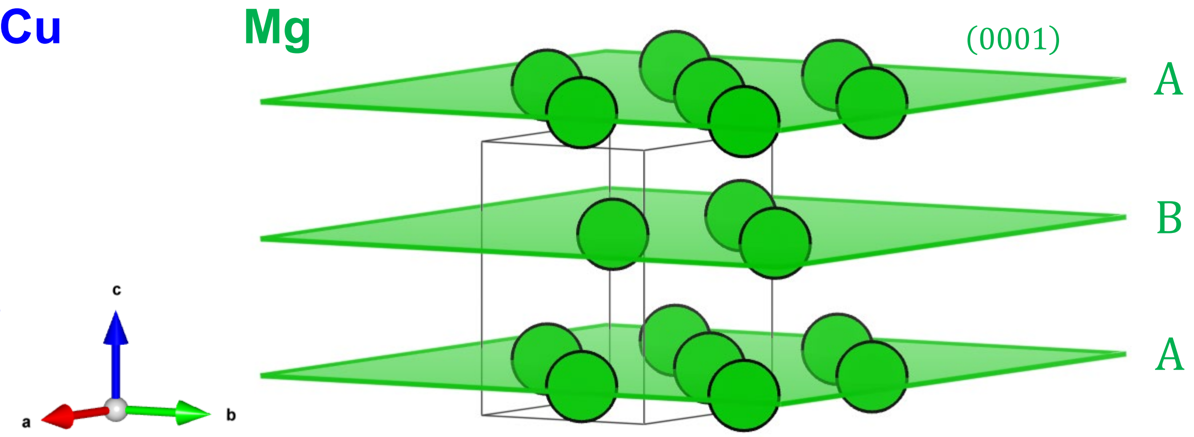
CSL with $\Sigma 5$:
$36.87°$ about $[001]$

The volume of the DSC unit cell is much smaller. In order to model deviations of these ideal sites, grain boundary dislocation are necessary. Due to the significantly smaller Burgers vectors, the grain boundary dislocations are dislocation in the DSC lattice.

Stacking Faults

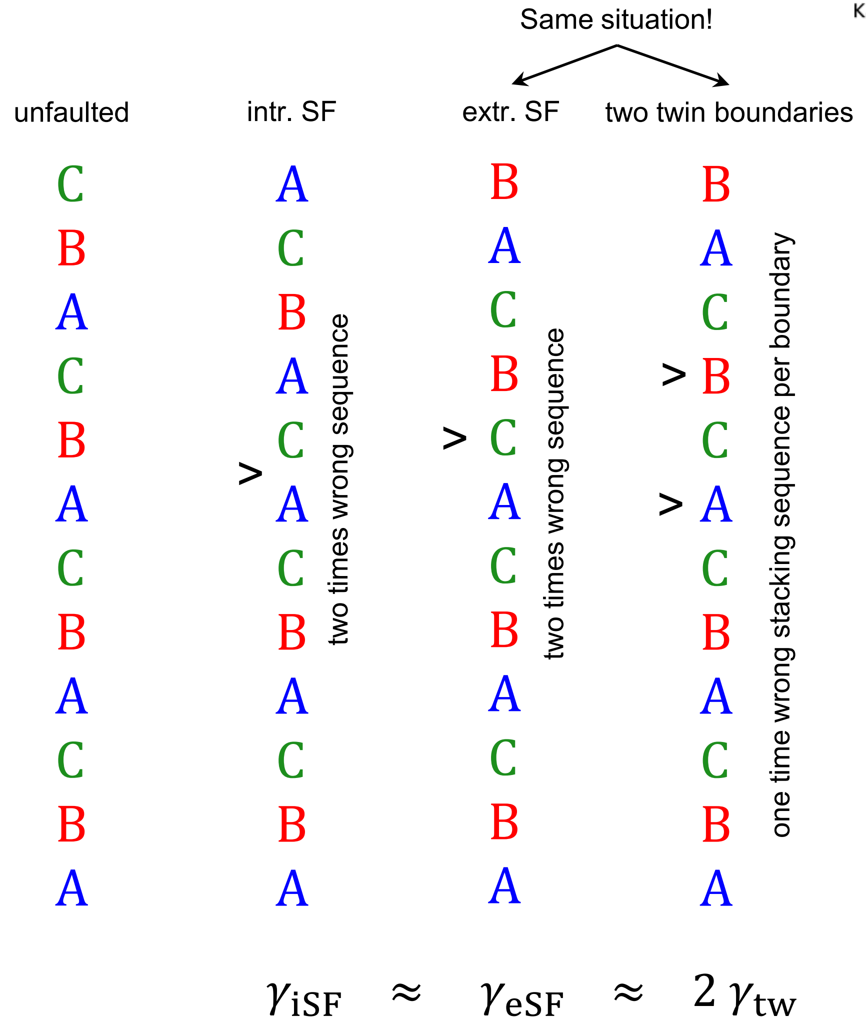
- All crystal structures are formed by specific stacking sequences of lattice planes (in general and valid for all kinds of planes, but mostly with complex sequences).
- In some crystal structures, metastable faults of the stacking sequences exist, e.g. fcc and hcp metals.
- In intermetallic compounds, the site occupation within the planes results in more complex versions of faults, e.g. antiphase boundary and complex faults.





Stacking Faults

- **In Cu structure type, the nearest neighbor (NN) interaction dominates.**
- Hence, for any close packed plane ABC, CBA and ACB are **ground state**.
- There is an **excess energy** needed to form ABA, CBC, CAC, BAB, BCB and ACA.



Same situation!

unfaulted	intr. SF	extr. SF	two twin boundaries
C	A	B	B
B	C	A	A
A	B	C	C
C	A	B	> B
B	C	> C	C
A	> A	A	> A
C	C	C	C
B	B	B	B
A	A	A	A
C	C	C	C
B	B	B	B
A	A	A	A

two times wrong sequence

two times wrong sequence

one time wrong stacking sequence per boundary

$$\gamma_{\mathrm{iSF}} \approx \gamma_{\mathrm{eSF}} \approx 2\,\gamma_{\mathrm{tw}}$$

Summary

- **Crystal defects can be classified according to their dimensionality.**
- **Complexity of crystals** leads to **various forms of each defect type**.
- There are **several interrelations between the different types** of crystal defects.