Karlsruhe Institute of Technology

Institute for Applied Materials

Plasticity

Lecture for “Mechanical Engineering” and “Materials Science and Engineering”
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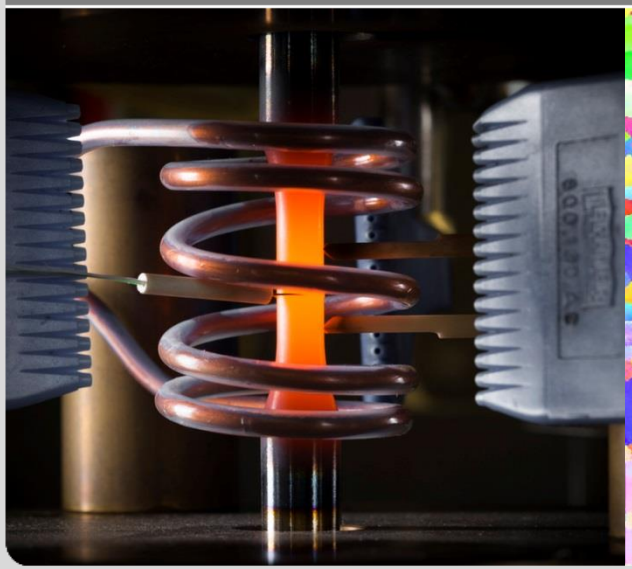
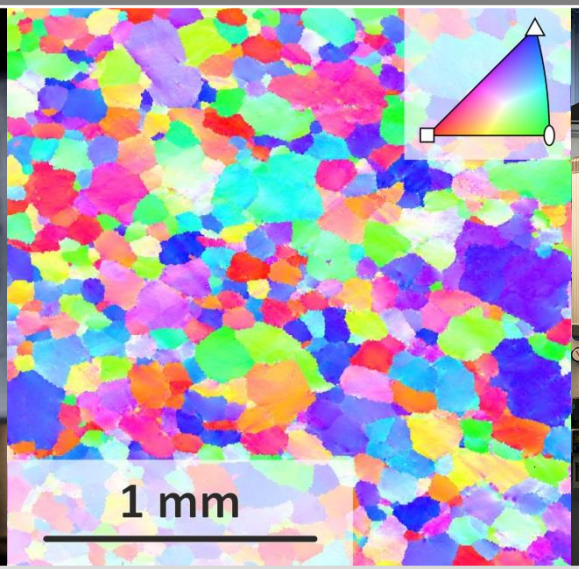
Version 22-04-27

Institute for Applied Materials (IAM-WK)





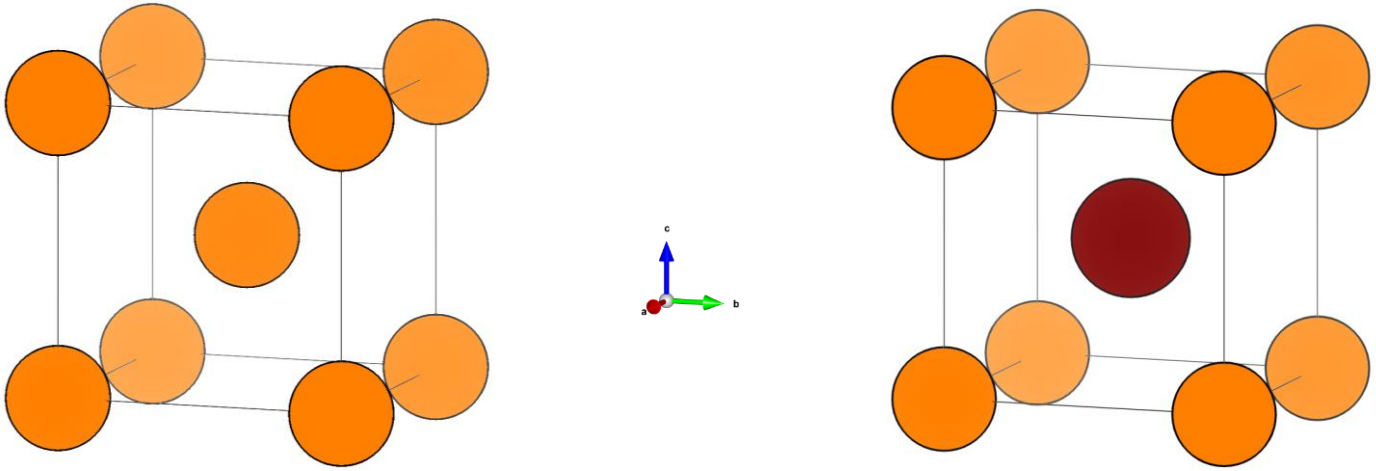
Topics

- Dislocations in Intermetallic Compounds
  - Comparison of A1, A2, and A3 metals alloys with ordered phases
  - Applying the stacking fault scheme to ordered alloys: antiphase boundaries and complex faults
  - Examples
    - B2
    - $L1_2$
  - Consequences

Remember Ch. 3c

- Most crystal structures of intermetallic compounds exhibit strong similarity to disordered metals. Hence, the structures can easily be described by the symmetry breaking and the introduction of order:

for example Fe und FeAl

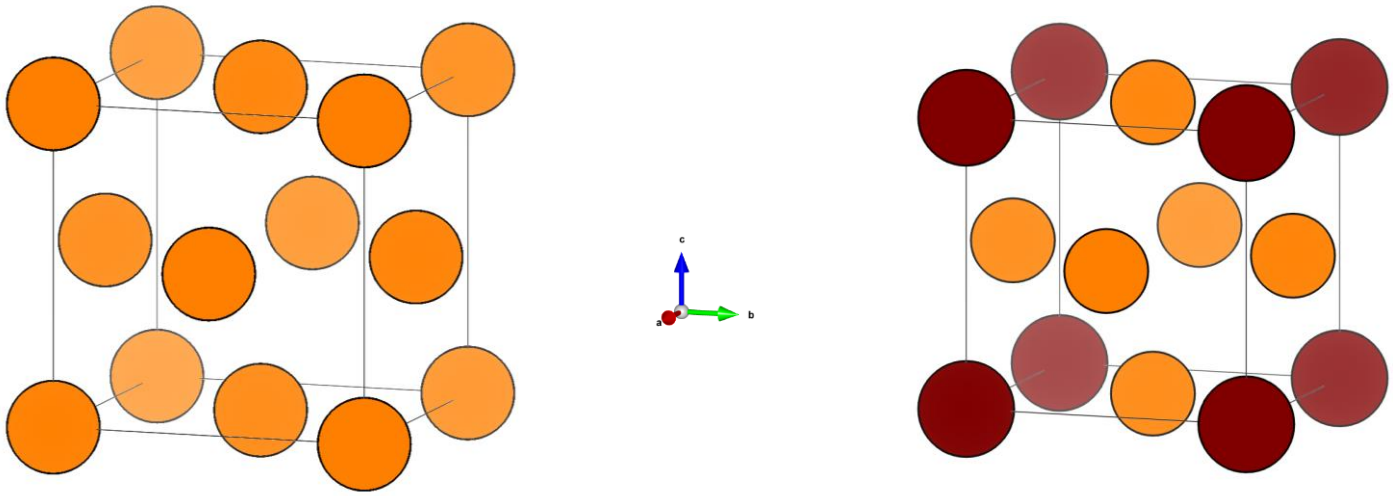


A2 **B2**

Remember Ch. 3c

- Most crystal structures of intermetallic compounds exhibit strong similarity to disordered metals. Hence, the structures can easily be described by the symmetry breaking and the introduction of order:

for example Ni und Ni_3Al

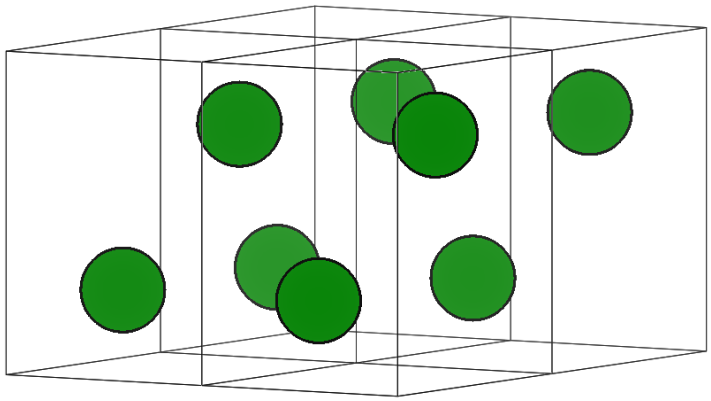


A1 **$L1_2$**

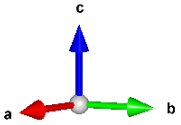
Remember Ch. 3c

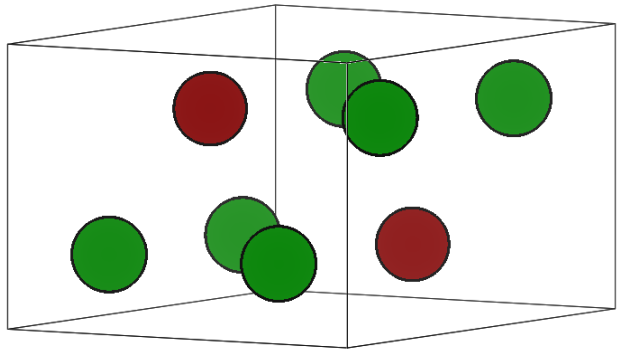
- Most crystal structures of intermetallic compounds exhibit strong similarity to disordered metals. Hence, the structures can easily be described by the symmetry breaking and the introduction of order:

for example Ti und Ti_3Al



A3





$D0_{19}$

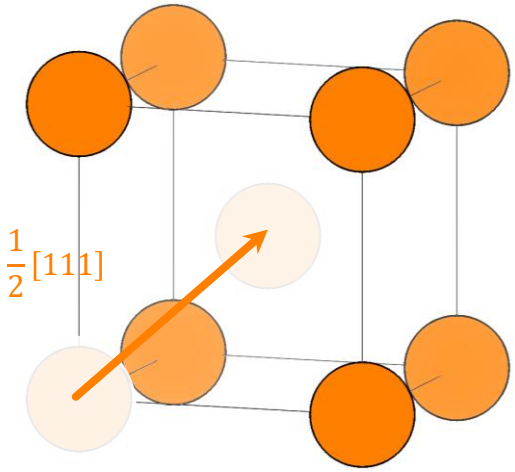
Note that the IUCr version of A3, the unit cell is rotated of 180° in comparison to this presentation!

Intermetallic Compounds

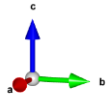
- We will use this analogy to deduce dislocation properties in these intermetallic compounds.
- It is important that any dislocation process should preserve the order in the compound. Otherwise, diffusion processes are necessary to recover order.

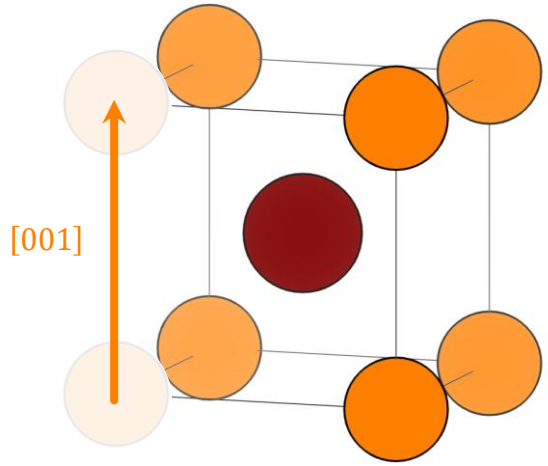
Intermetallic Compounds: B2

- Burgers vectors, shortest full lattice vector:



A2





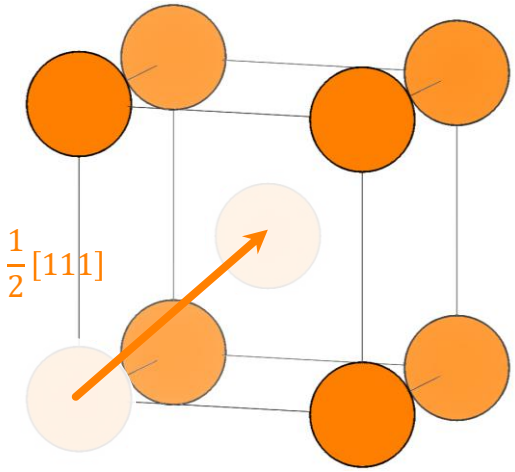
B2

$\frac{1}{2}\langle 111\rangle$ is the shortest lattice vector in the primitive, trigonal unit cell of A2.

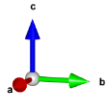
By the introduction of order in B2, the symmetry is broken and the primitive unit cell is now indeed simple cubic with a two atomic crystallographic basis (one of the atoms on the corner, one in the center of the unit cell). Hence, the shortest Burgers vector preserving the structure is $\langle 100\rangle$.

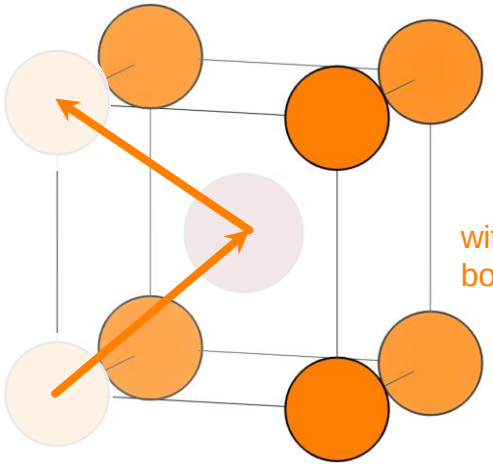
Intermetallic Compounds: B2

- Burgers vectors, dissociation:



A2



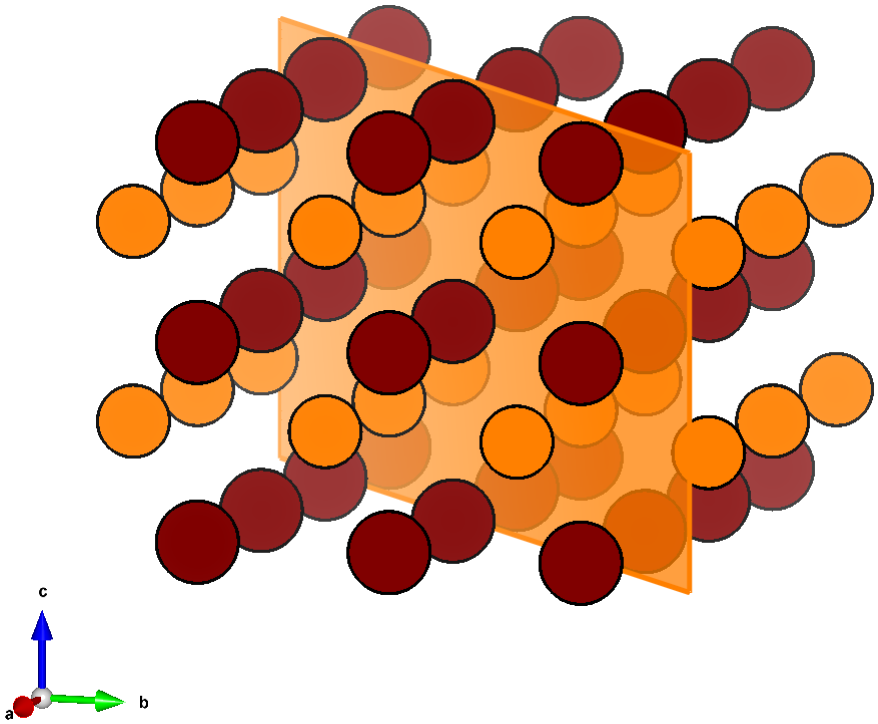


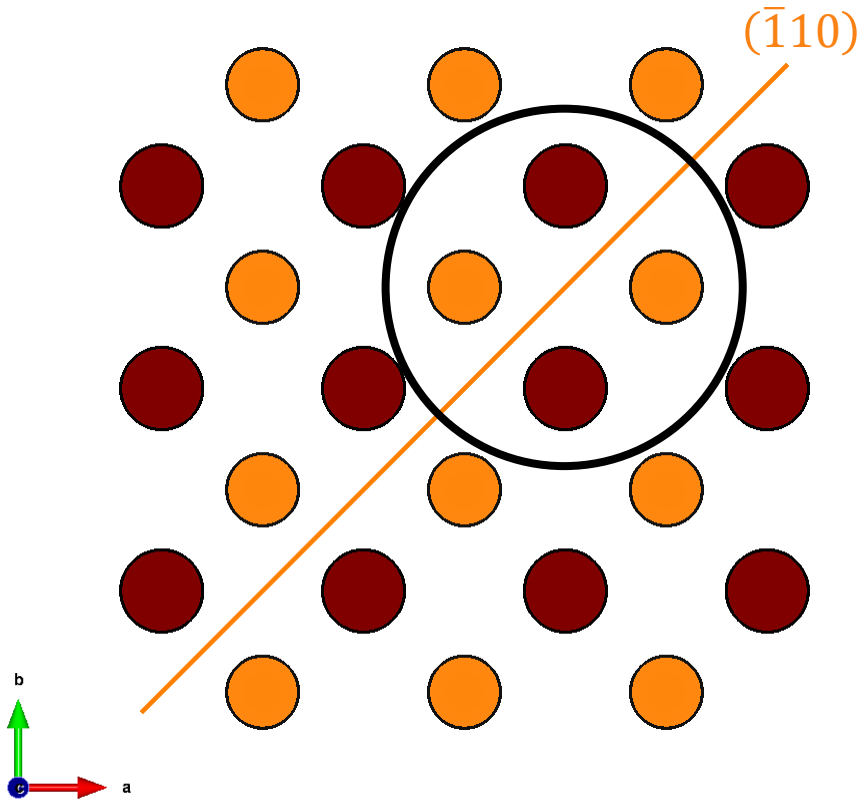
B2

Similar to what was seen in A1 metals, shorter Burgers vectors can be achieved by dissociation. A metastable planar fault of low energy is then necessary: in this case an antiphase boundary.

Intermetallic Compounds: B2

- Perfect B2 lattice, **all NN bonds are of A-B type**!



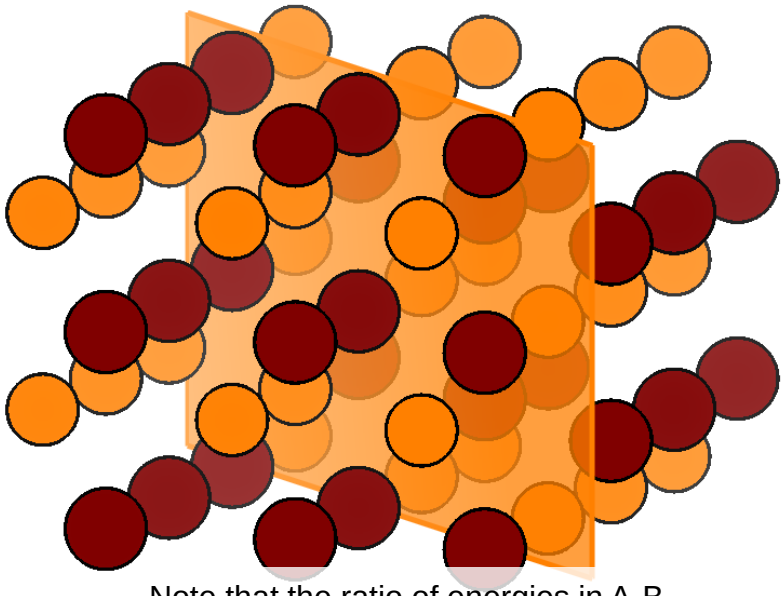


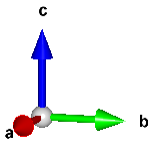
$[00\bar{1}]$ top view

Intermetallic Compounds: B2

- Introduction of an antiphase boundary by $\frac{1}{2}[111]$ displacement within $(\bar{1}10)$.

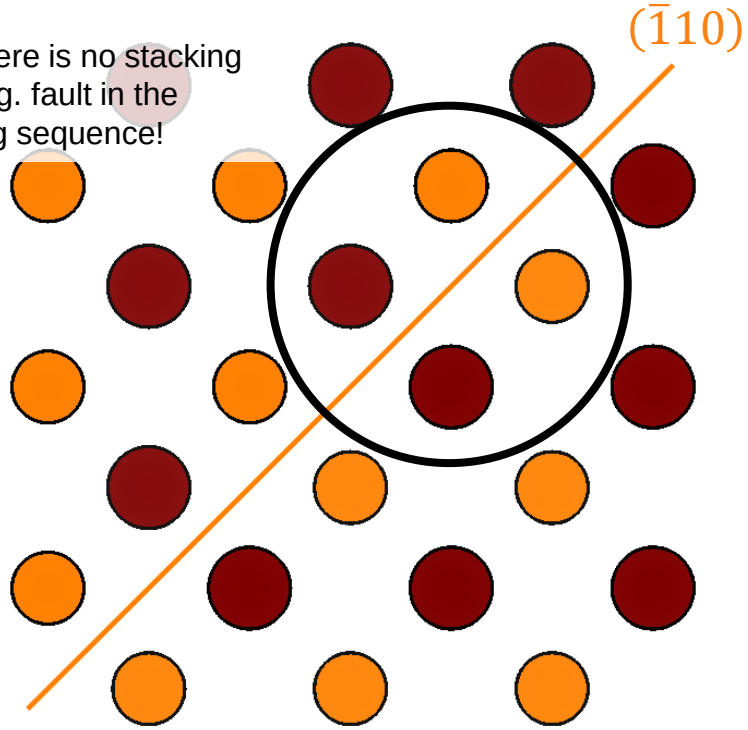
  The energy of the defect is determined by the excess energy of B-B and A-A bonds.

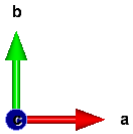




Note that the ratio of energies in A-B bonds vs. A-A and B-B bonds is well described by the exchange energy introduced in the fundamental lectures (like “Metalle”)

Note there is no stacking fault, e.g. fault in the stacking sequence!





$[00\bar{1}]$ top view

Intermetallic Compounds: B2

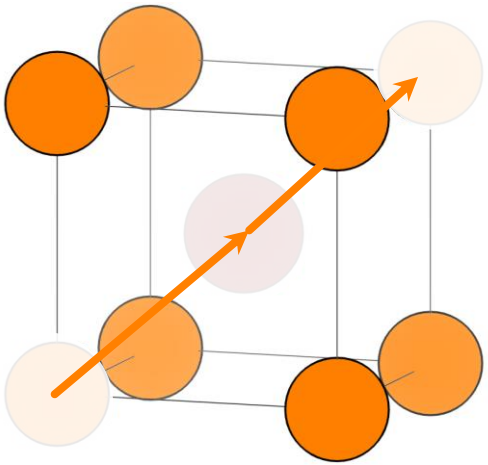
- In general, slip systems with either $\langle 111 \rangle$ or $\langle 001 \rangle$ **slip directions** are found in most B2 compounds.
- It significantly **depends on the tendency for ordering** (binding energy of A-B vs. A-A and B-B):
  - $\langle 001 \rangle$ (mostly with $\{100\}$) **when strong tendency for order**
  - $\langle 111 \rangle$ (mostly with $\{1\bar{1}0\}$) **when low tendency for order**
- In some systems, a **transition** from $\langle 111 \rangle$ to $\langle 001 \rangle$ is observed for **increasing temperature**.
- **Additional influences** are arising from:
  - exact antiphase boundary energy
  - deviations from 1:1 stoichiometry by constitutional point defects
  - orientation of mechanical load

Intermetallic Compounds: B2

- Burgers vectors, other possibilities and dissociation:

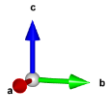
Note that there are two possibilities of dislocation dissociation which might lead to $\frac{1}{2}[111]$ dislocations:

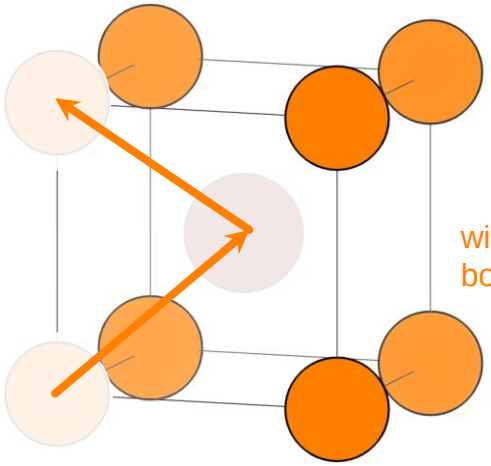
$2 \cdot \frac{1}{2}[111]$ with anti-phase boundary



B2

Co-linear dissociation of a the long space diagonal. There is no distinct plane for the planar fault!





$2 \cdot \frac{1}{2}[111]$ with anti-phase boundary

B2

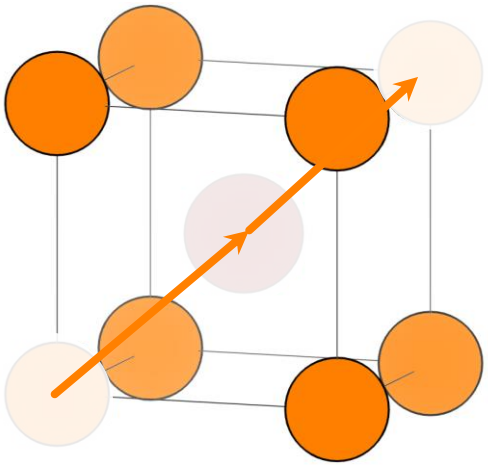
Planar dissociation of a $\langle 001 \rangle$ dislocation. The planar fault can only be of $\{\bar{1}10\}\frac{1}{2}\langle 111 \rangle$ type (see slides before).

Intermetallic Compounds: B2

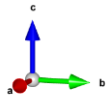
- Burgers vectors, other possibilities and dissociation:

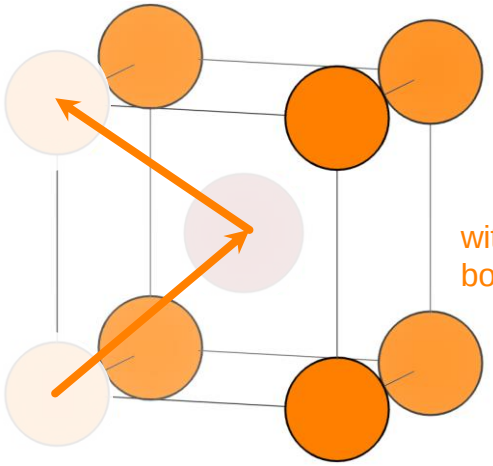
Note that there are two possibilities of dislocation dissociation which might lead to $\frac{1}{2}[111]$ dislocations:

$2 \cdot \frac{1}{2}[111]$ with anti-phase boundary



B2





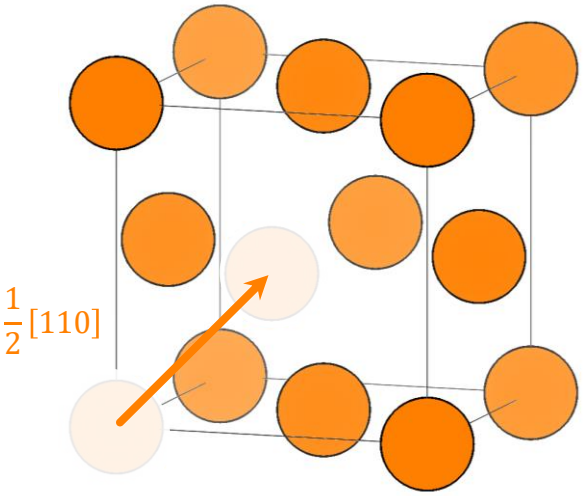
B2

$2 \cdot \frac{1}{2}[111]$ with anti-phase boundary

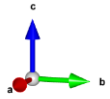
Different planes of the planar fault change the ratio of A-B to A-A and B-B bonds!

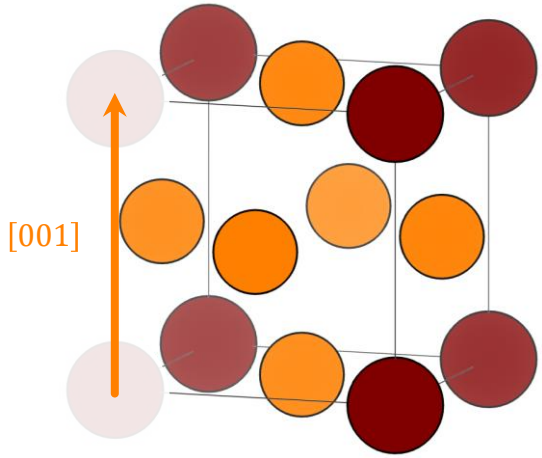
Intermetallic Compounds: $L1_2$

- Burgers vectors, shortest full lattice vector:



A1





$L1_2$

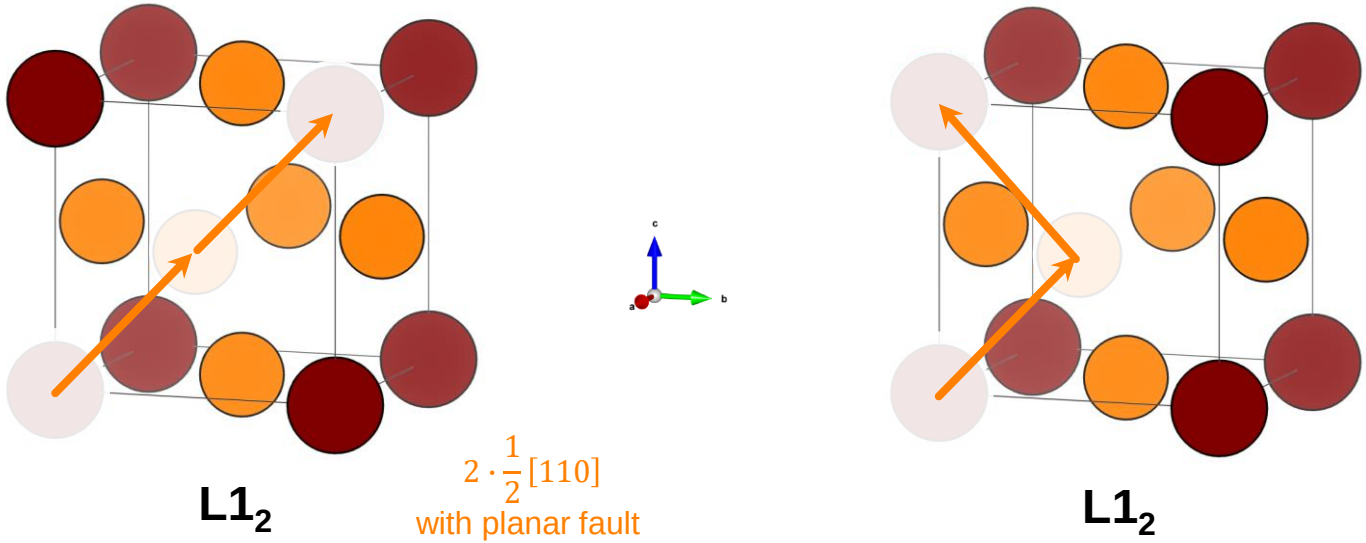
Again, the unit cell is simple cubic. The crystallographic basis consists of four atoms. The shortest lattice vector is $\langle 001 \rangle$.

Intermetallic Compounds: $L1_2$

- In most cases, slip is found for $\{111\}\langle 1\bar{1}0\rangle$ system. Sometimes $\{001\}\langle 1\bar{1}0\rangle$ are identified.
- There are **additional influences** by:
  - Temperature
  - Antiphase boundary energy
  - Deviations from exact stoichiometry
  - Orientation of mechanical loading

Intermetallic Compounds: $L1_2$

- Burgers vectors, other possibilities and dissociation:

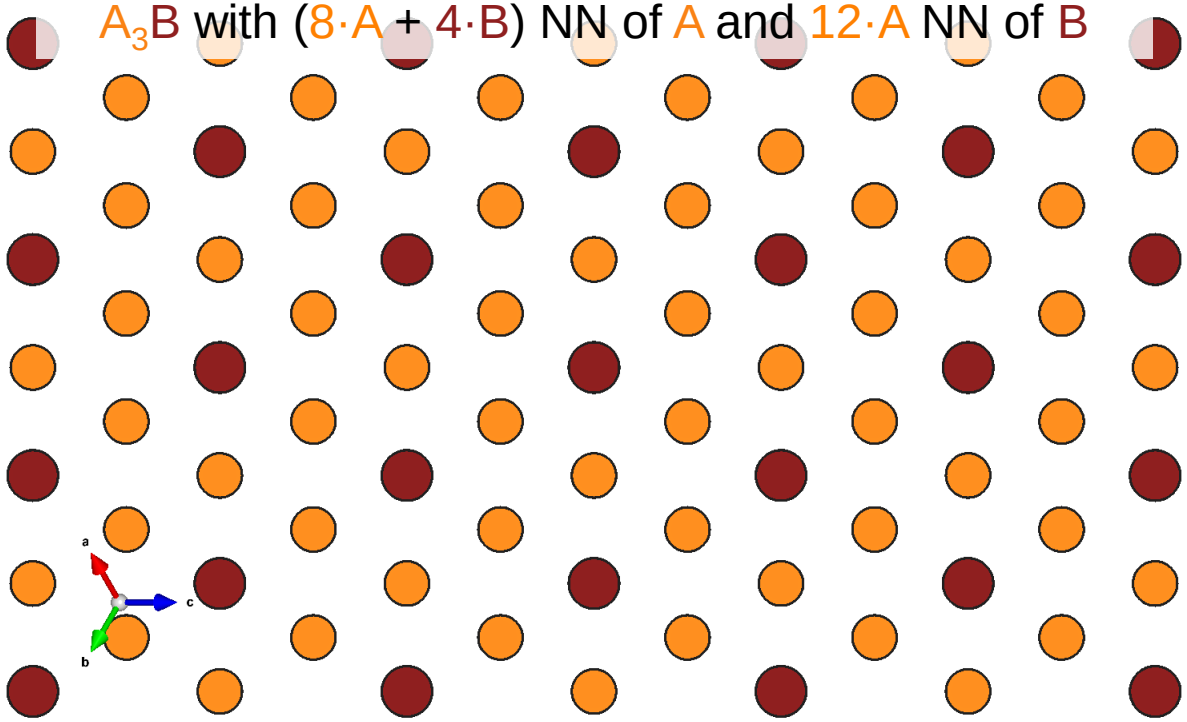


Co-linear and co-planar $\frac{1}{2}\langle 110 \rangle$ Burgers vectors.

Intermetallic Compounds: $L1_2$

- The analysis is more challenging for $L1_2$ since there are A-B as well as A-A and B-B bonds in the undistorted structure.
- $L1_2$ is a super structure of A1. Therefore, there are 12 NN:

top view on {111}



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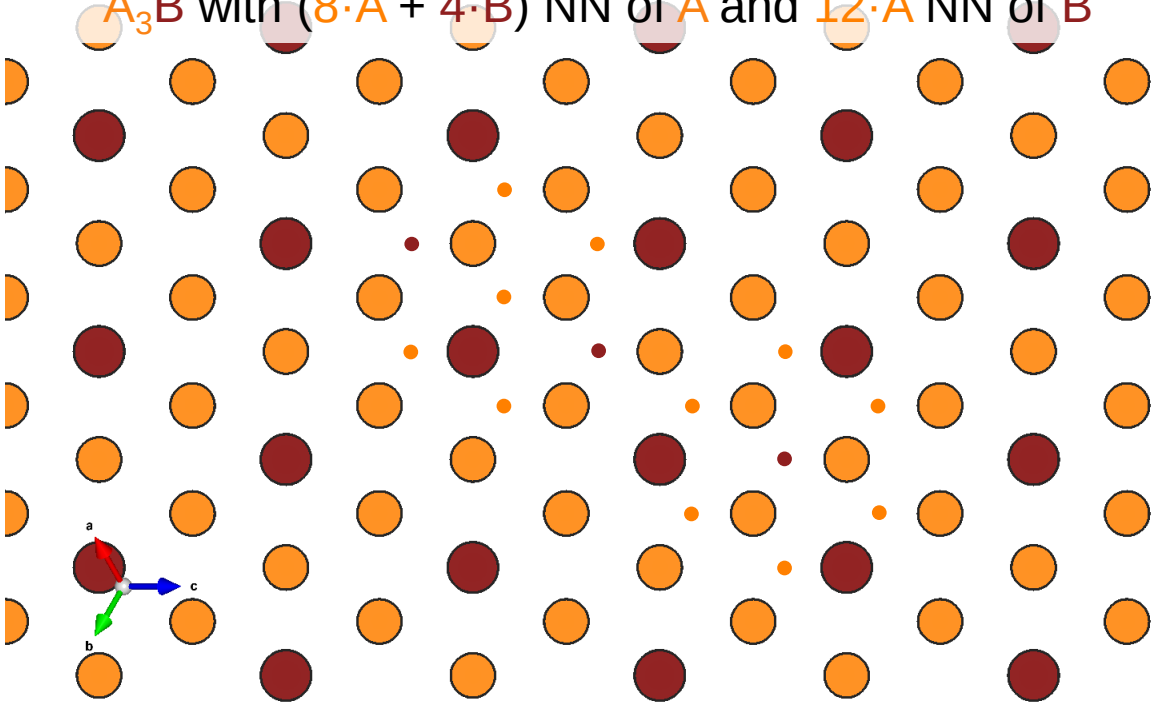
A_3B with (8·A + 4·B) NN of A and 12·A NN of B

top view on {111}



one plane below

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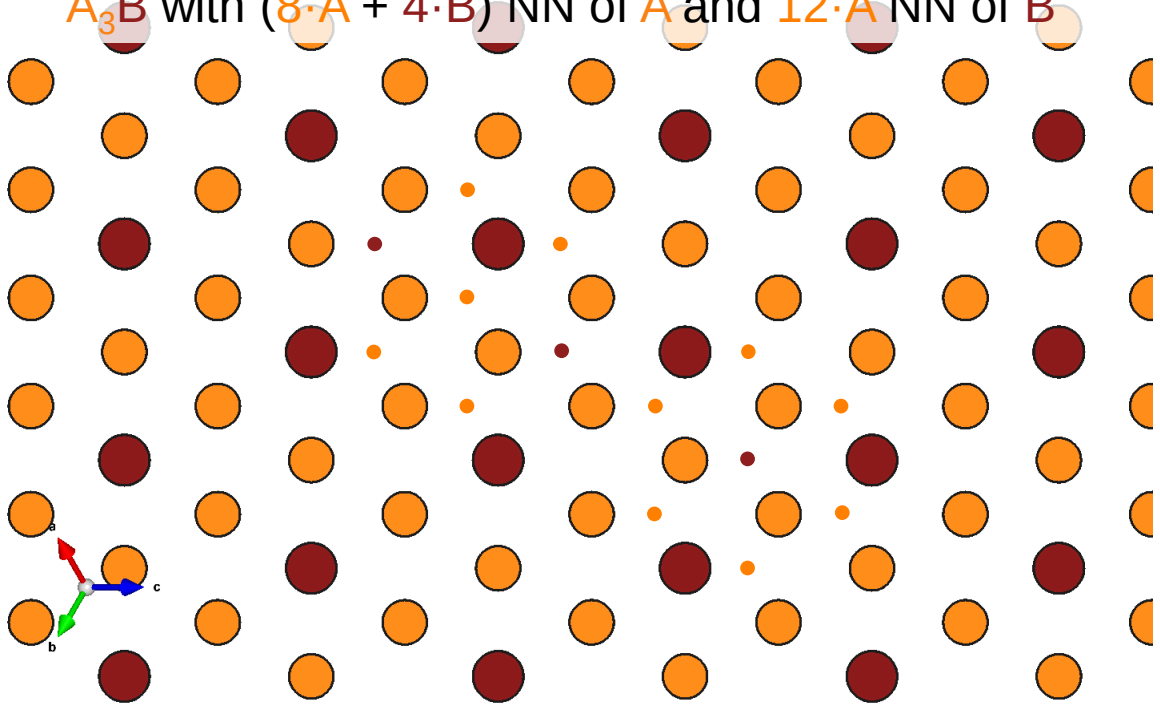
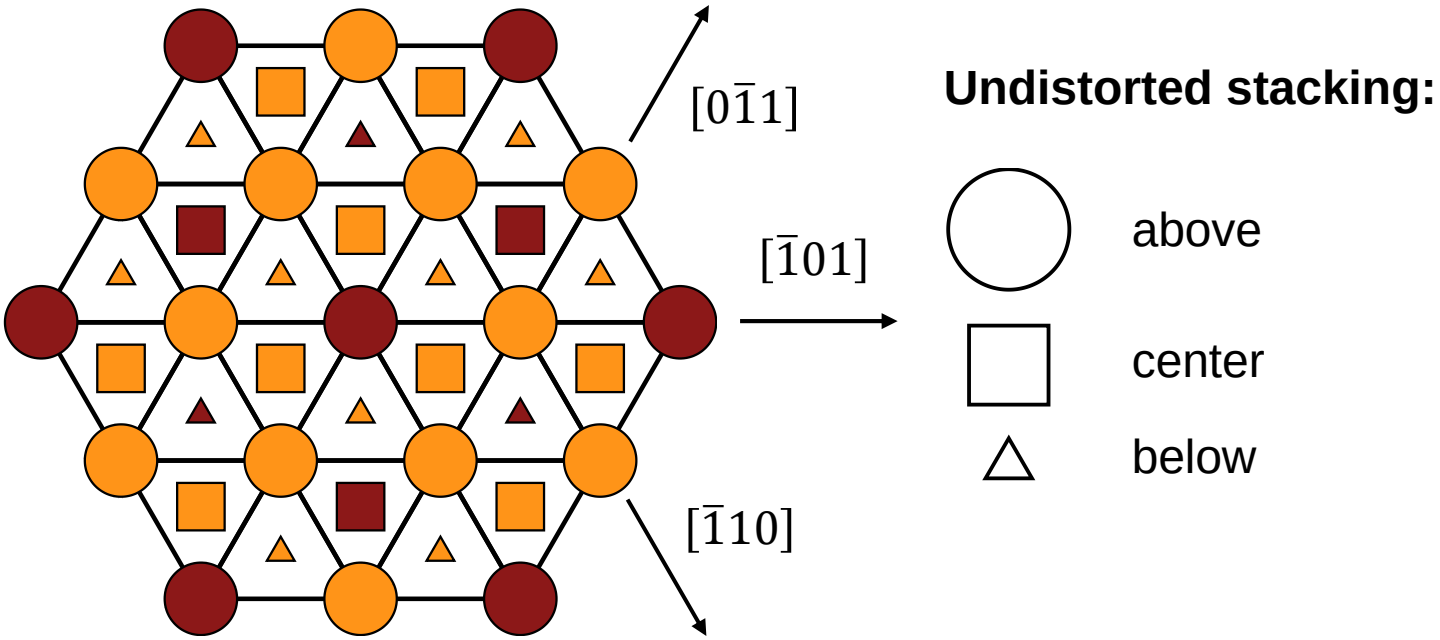
top view on {111}



one plane above

Intermetallic Compounds: $L1_2$

- Faults can be: stacking faults, antiphase boundaries or mixtures of both (complex faults)!



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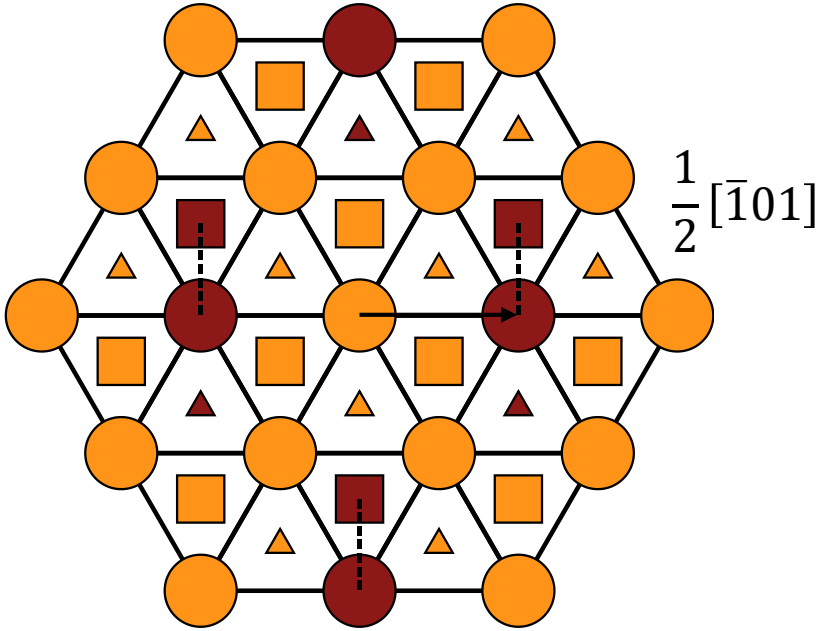
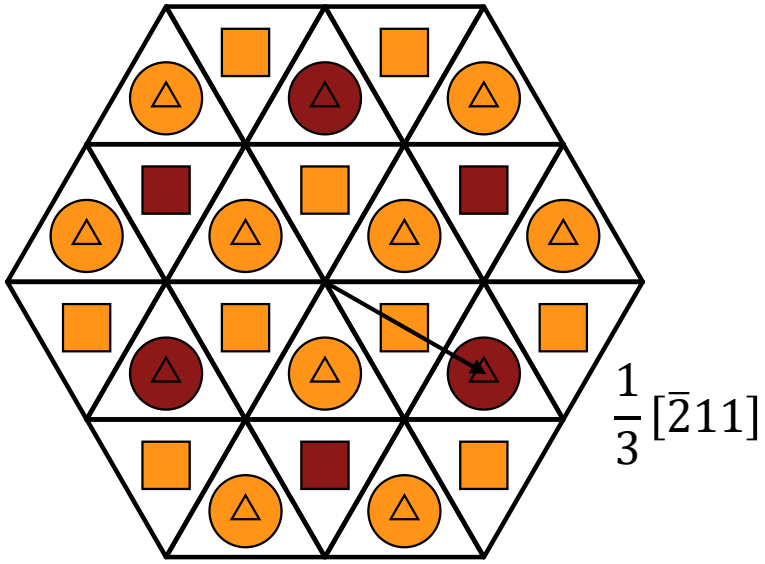


Anti-phase boundary by displacement of the upper layer about $\frac{1}{2}[\bar{1}01]$. The center B atoms now have B-B instead of A-B bonds.

Intermetallic Compounds: $L1_2$

- Faults can be: stacking faults, antiphase boundaries or mixtures of both (complex faults)!

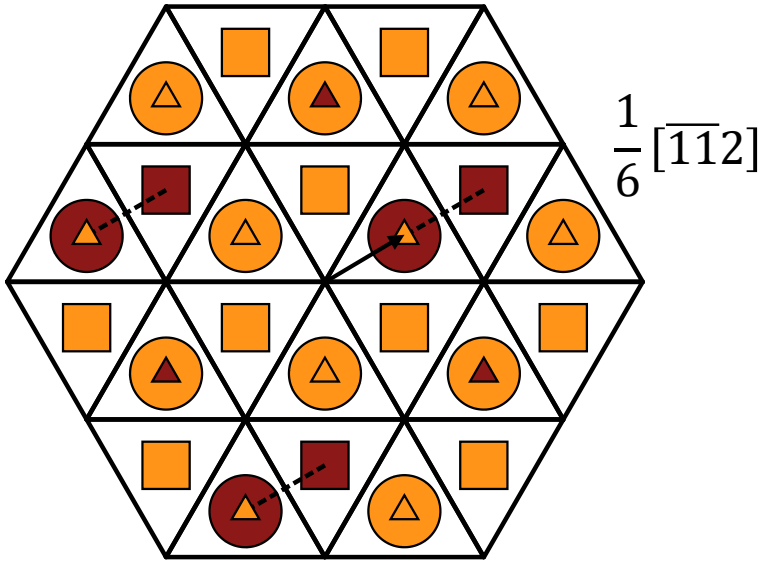


Intrinsic stacking fault displacment of the upper plane about $\frac{1}{3}[\bar{2}11]$.

There is no change in NN bonds.
There is a missing plane in the stacking sequence!

Intermetallic Compounds: $L1_2$

- Faults can be: stacking faults, antiphase boundaries or mixtures of both (complex faults)!



$\frac{1}{6}[\overline{1}\overline{1}2]$

Complex Fault by displacement along $\frac{1}{6}[\overline{1}\overline{1}2]$. Both, number of bonds and stacking sequence is changed!

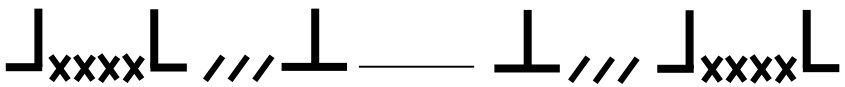
Intermetallic Compounds: $L1_2$

- There are mainy possible dissociation scenarios in $L1_2$:

$$[\bar{1}01] \rightarrow \frac{1}{2}[\bar{1}01] + \frac{1}{2}[\bar{1}01]$$

$$[\bar{1}01] \rightarrow \frac{1}{3}[\bar{2}11] + \frac{1}{3}[\overline{11}2]$$

$$[\bar{1}01] \rightarrow \frac{1}{6}[\overline{11}2] + \frac{1}{6}[\bar{2}11] + \frac{1}{6}[\bar{2}11] + \frac{1}{6}[\overline{11}2]$$



etc.

etc.

- In reality, non-planar dissociations appear!

Intermetallic Compounds: $L1_2$

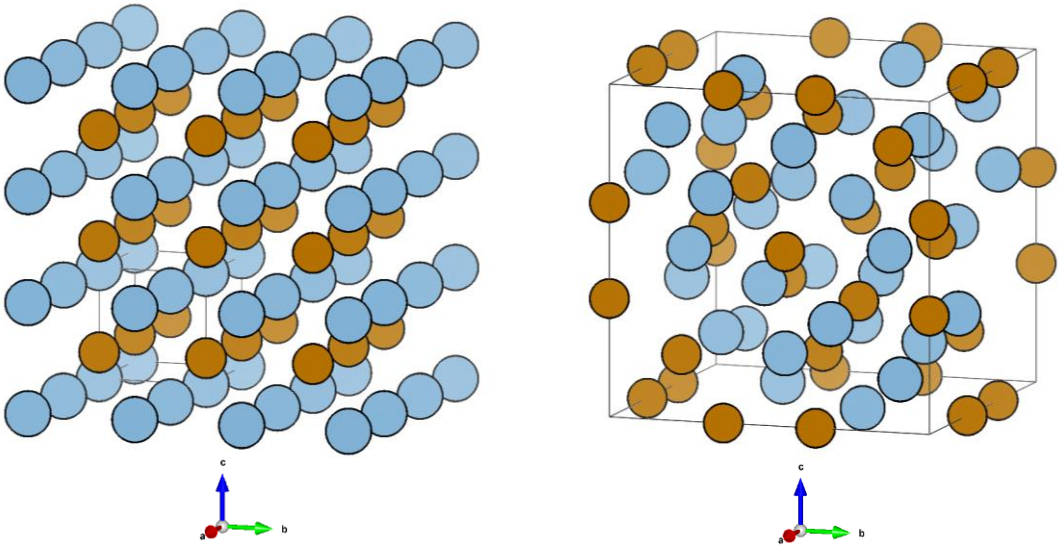
- For A1, we have seen that:
  - Cross-slip is controlled by dissociation. Cross-slip determines the work-hardening behavior due to the contribution to dynamic recovery.
  - Work-hardening is additionally altered by the formation of sessile dislocation reaction products.
- **Both consideration can directly be transferred to $L1_2$ structures.** Due to the higher number of possible dissociations and faults, scenarios for cross-slip and lock formation are manifold.

Consequences

- In some technically relevant materials like super alloys, the ordered phases form coherent precipitates in the disordered matrix. The penetration process of dislocations form the disordered matrix into the particles is important for the assessment of the strengthening contributions by the particles. Here, the direct comparison of Burgers vectors, dissociations and faults in the disordered and ordered alloys is a key task: short Burgers vectors in the disordered structures often lead to faults in the ordered structure.

Consequences

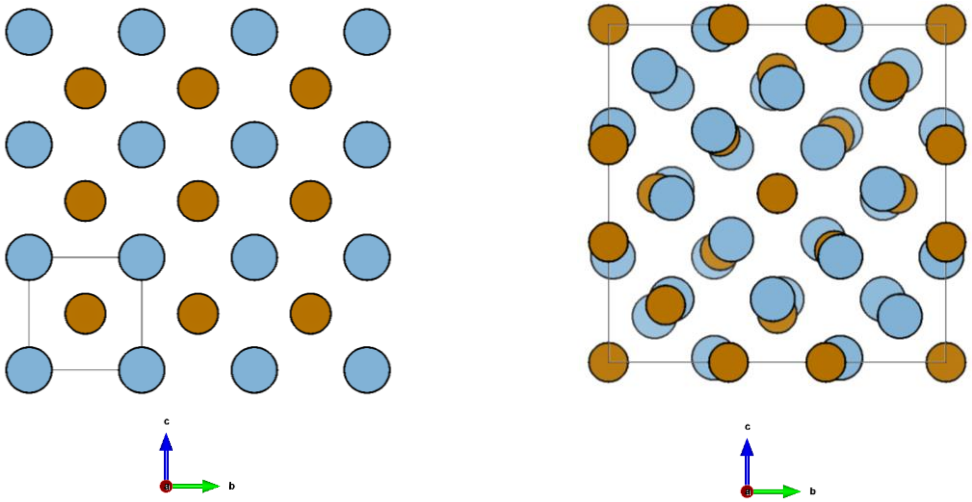
- Order is just an example, for the analogy treatment. Additionally, the atoms can be displaced from the ideal positions in the disordered structures.



FeAl (B2) and Fe_5Al_8 ($D8_2$)

Consequences

- Order is just an example, for the analogy treatment. Additionally, the atoms can be displaced from the ideal positions in the disordered structures.

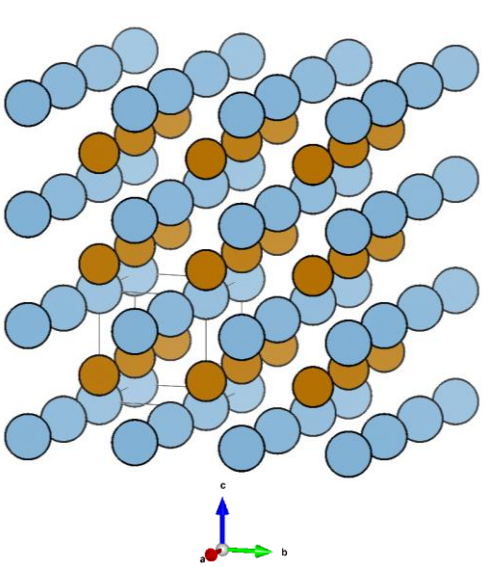
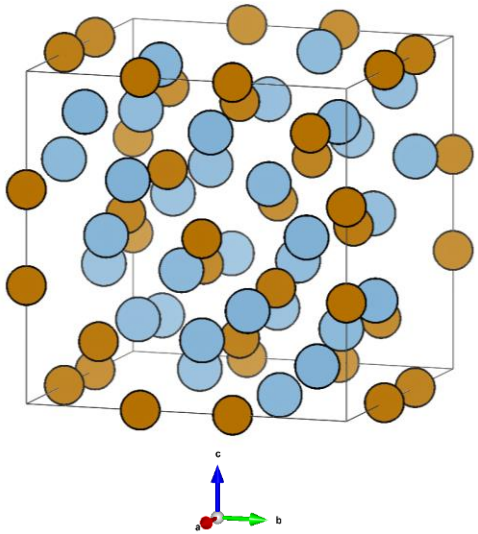
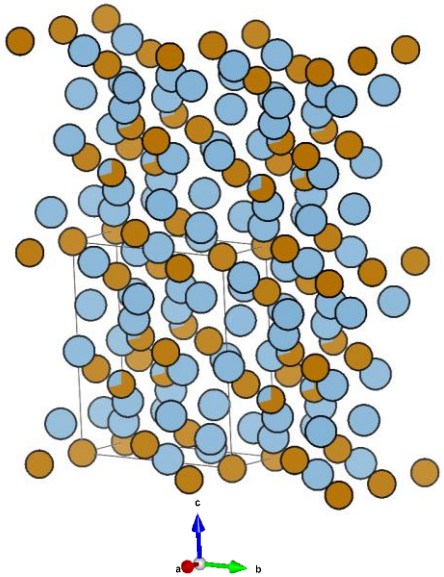


FeAl (B2) and Fe_5Al_8 ($D8_2$)

Cu_5Zn_8- is a 3x3x3 super structure of A2 with additional displacements of the atoms.

Consequences

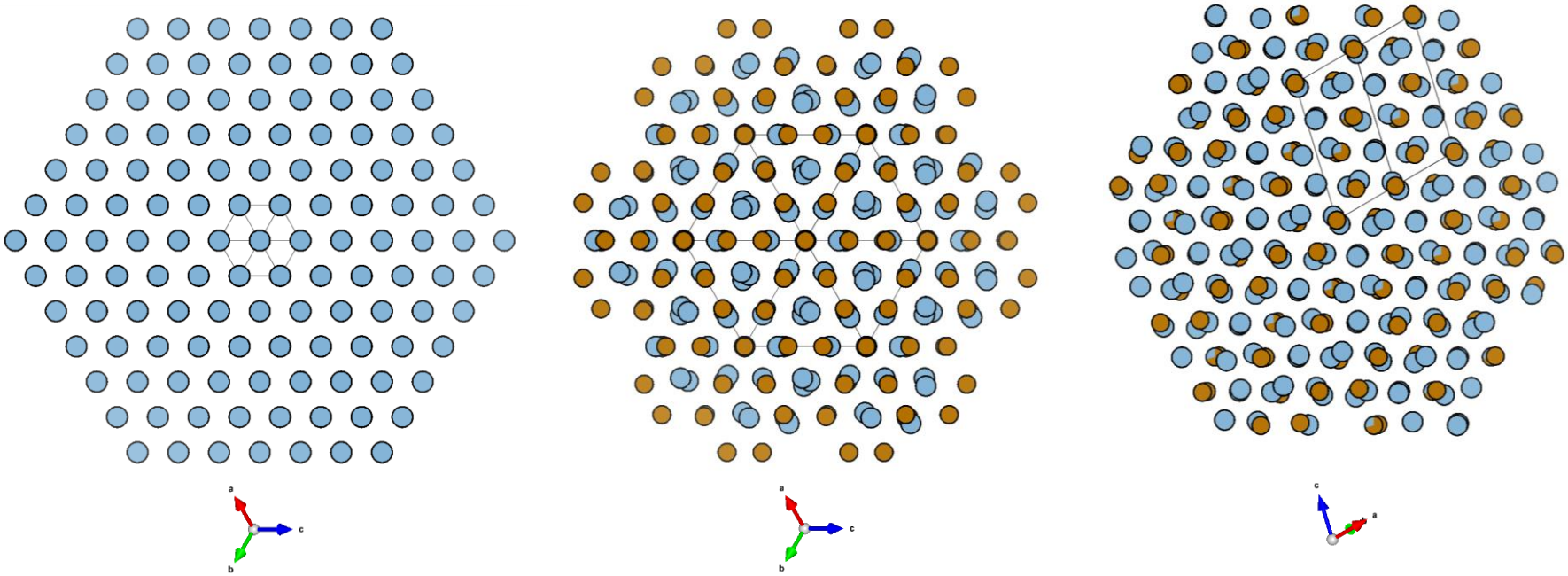
- Order is just an example, for the analogy treatment. Additionally, the atoms can be displaced from the ideal positions in the disordered structures.

FeAl (B2) and Fe_5Al_8 ($D8_2$) and triclinic $FeAl_2$

Consequences

- Order is just an example, for the analogy treatment. Additionally, the atoms can be displaced from the ideal positions in the disordered structures.



Even in very complex phases, it is a matter of view point!

Consequences

- Constitutional and structural vacancies can have significant influence on the deformation behavior of intermetallic compounds.
- Only few examples exist, where plastic deformation is completely different from disordered alloys, e.g. by deformation on Kagome layers or synchro-shear mechanism.

Summary

- The analyses of dislocation structures in intermetallic compounds is in many cases based on the direct comparison to the disordered alloys and by utilizing the order relationship of both.
- The dissociation of dislocations results in stacking faults, antiphase boundaries of complex faults.
- The various possibilities of dissociation and lock formation significantly contribute to work-hardening behavior of the phases.
- In most cases details depend on: temperature, loading direction, stoichiometry, etc.