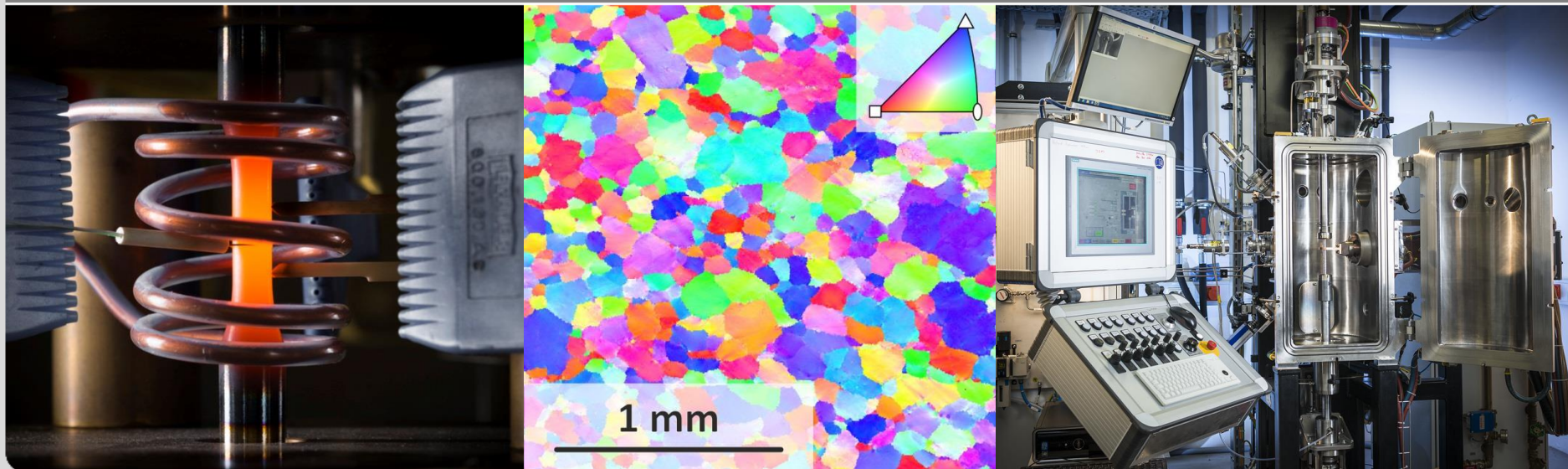


# Plasticity

Lecture for “Mechanical Engineering” and “Materials Science and Engineering”  
Dr.-Ing. Alexander Kauffmann (Bldg. 10.91, R. 375)  
Prof. Martin Heilmaier (Bldg. 10.91, R. 036)

Version 22-07-14

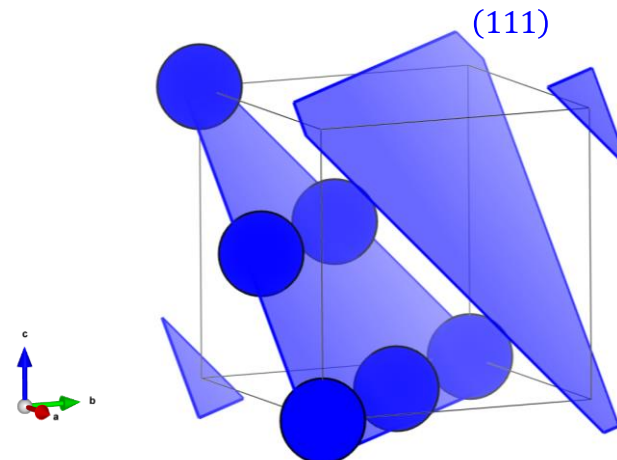
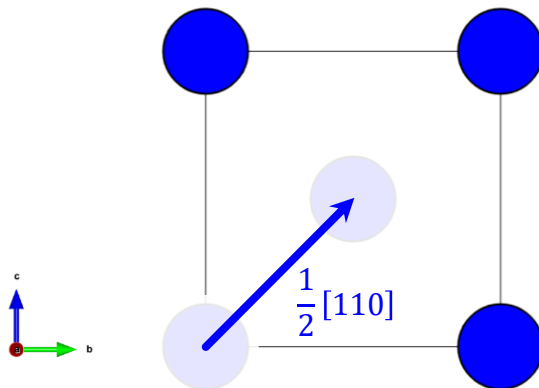
Institute for Applied Materials (IAM-WK)



- Dislocations in Metals and Alloys: A1
  - Octahedral Slip Systems
  - Thompson Tetrahedron
  - Undissociated Dislocations
  - Shockley and Frank Partial Dislocations
  - Stacking Faults and Twin Boundaries
  - Cross Slip
  - Locks

# Strukturbericht Designation A1

- **Face centered cubic metals and alloys are closed packed.** The closed packed planes are  $\{111\}$ . The shortest distance between atoms is  $\frac{1}{2}\langle 110 \rangle$ . (Remember: use of the conventional cell here.)



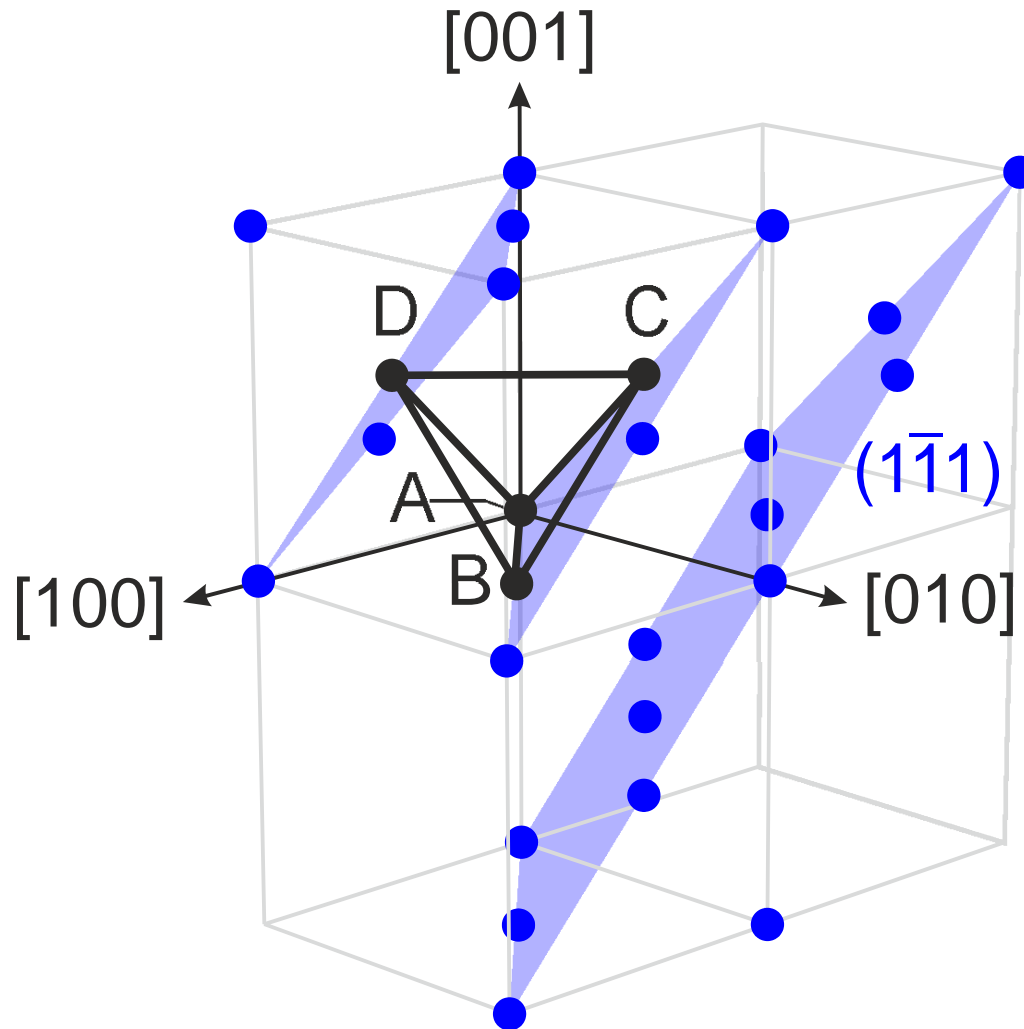
# Octahedral Slip System

- $\{111\} \frac{1}{2} \langle 1\bar{1}0 \rangle$  slip systems are referred to as **octahedral slip systems**.
- In fcc metals and alloys, **slip on non-octahedral systems is assumed to be not possible**. Any **reaction products** with combinations of Burgers vectors and slip planes (given by the Burgers vector and the line sense) which do not belong to the octahedral slips systems are assumed to be **sessile**.
- There are various short notations in literature to describe octahedral systems and reactions on these systems available. The **Thompson tetrahedron** is by far the most common. Anyhow, the use of it is declining.

# Thompson Tetrahedron

- **The edges of the Thompson tetrahedron are given by the connection of four nearest neighbors in the A1 crystal structure.**
- Important to note here:
  - The Thompson tetrahedron is no unit cell! It is not possible to obtain a perfect crystal by translation symmetry or application of other symmetry operations on it!
  - The Thompson tetrahedron connects nearest neighbors and not corners of the conventional unit cell.
  - Often missed in literature: Similar to what was seen for the Burgers circuits, the Thompson tetrahedron treatment contains certain unambiguosness as long as the slip to crystal is not explicitly defined. It is important for the distinct atomic arrangement if slip occurs outside the Thompson tetrahedron (often implicitly assumed) or inside. Many reaction are possible by vector considerations but impossible due to the atomic arrangement resulting from that.
- **The corners are denoted by Latin capital letters: A, B, C, D. The Burgers vectors of undissociated dislocations are duplets of Latin capital letters. The slip planes are triplets of Latin capital letters.**

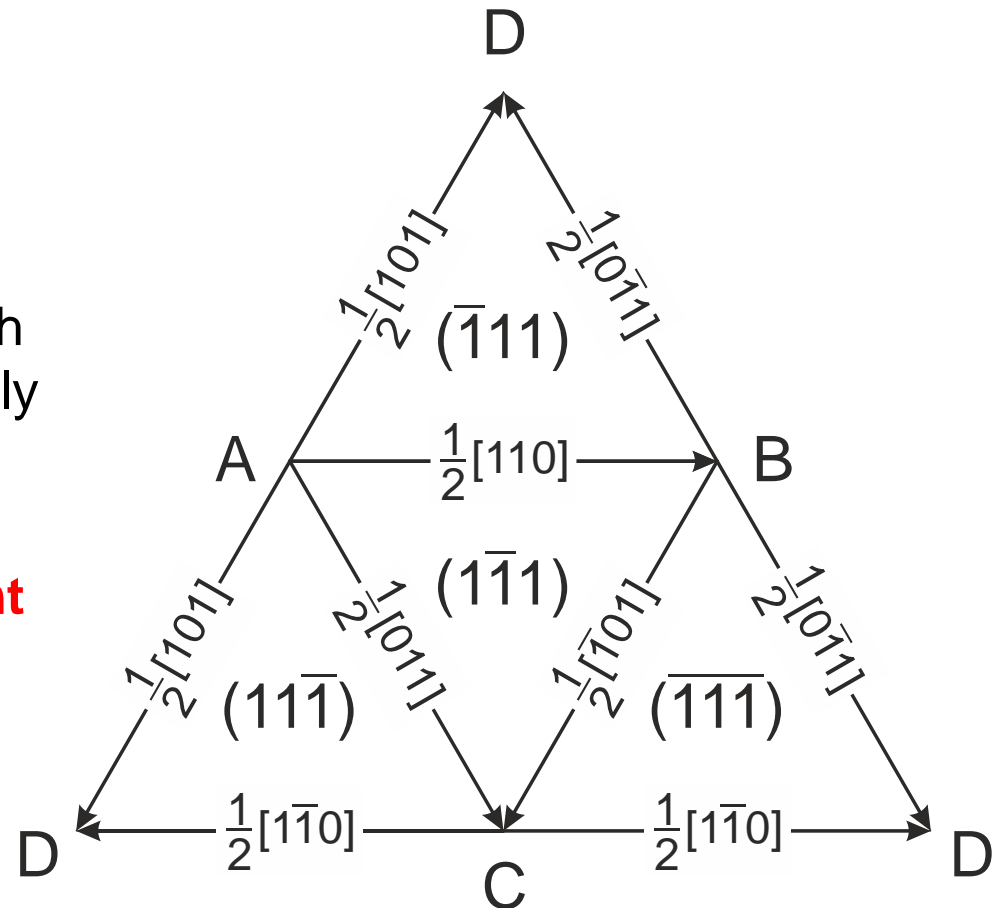
# Thompson Tetrahedron



A. Kauffmann: „Gefügeverfeinerung durch mechanische Zwillingsbildung in Kupfer und Kupfermischkristalllegierungen“, Diss. TU Dresden (2014)

# Thompson Tetrahedron

- **The flat projection of the tetrahedron is useful.**
- There are four slip planes with three slip directions each. Only two of them are linear independent.
- **There are eight independent slip systems.**



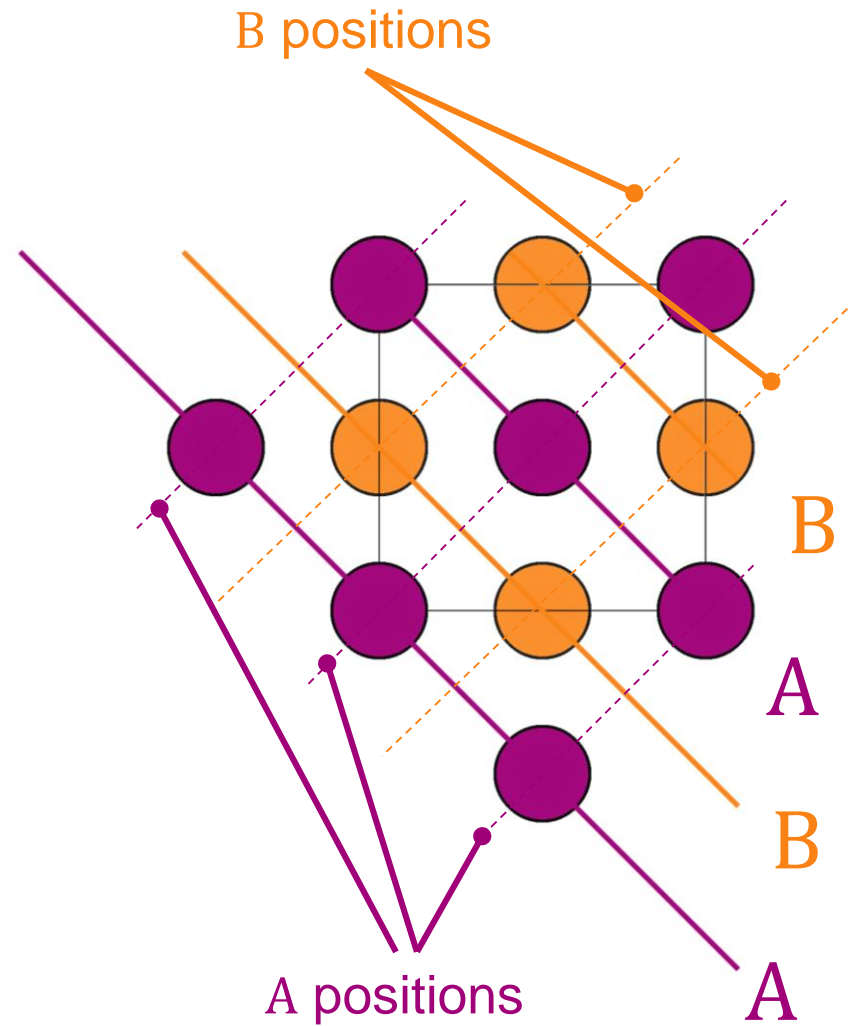
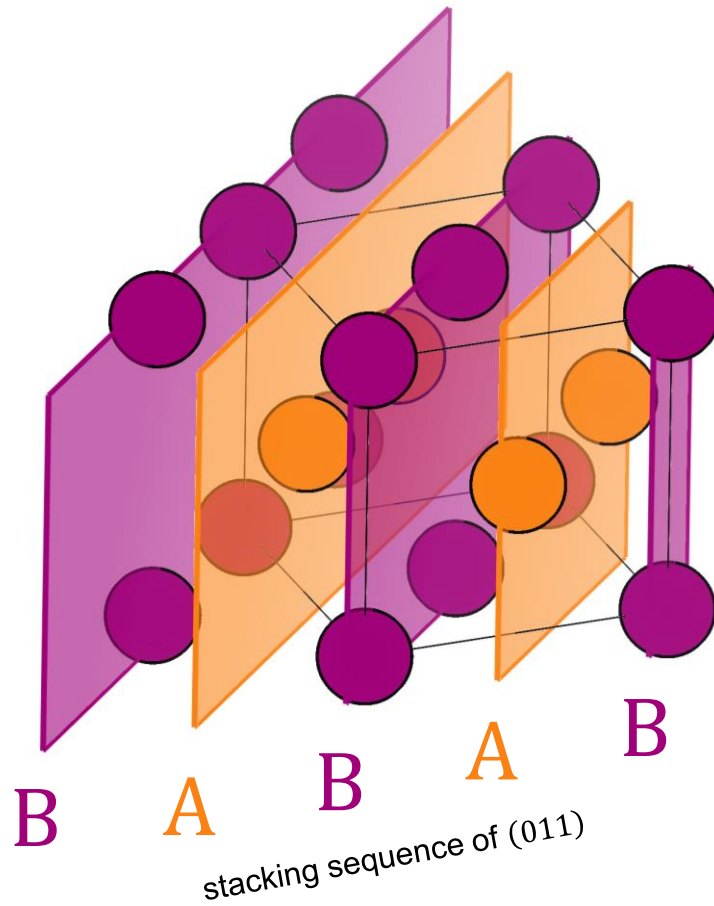
# Undissociated Dislocations

- The undissociated edge dislocation is characterized by following vectors:
  - Slip plane normal:  $\mathbf{n} = (1\bar{1}1)$ , ABC
  - Burgers vector:  $\mathbf{b} = \frac{1}{2}[011]$ , AC
  - Line vector:  $\mathbf{s} = \frac{1}{\sqrt{6}}[21\bar{1}]$ ,  $\delta B$
  - Extra half-plane:  $(011)$
- The extra half-planes of  $\{110\}$ -type exhibit following stacking sequence: ... ABABAB .... Hence, the undissociated edge dislocation is built up from two additional  $\{110\}$  planes to preserve the stacking sequence!

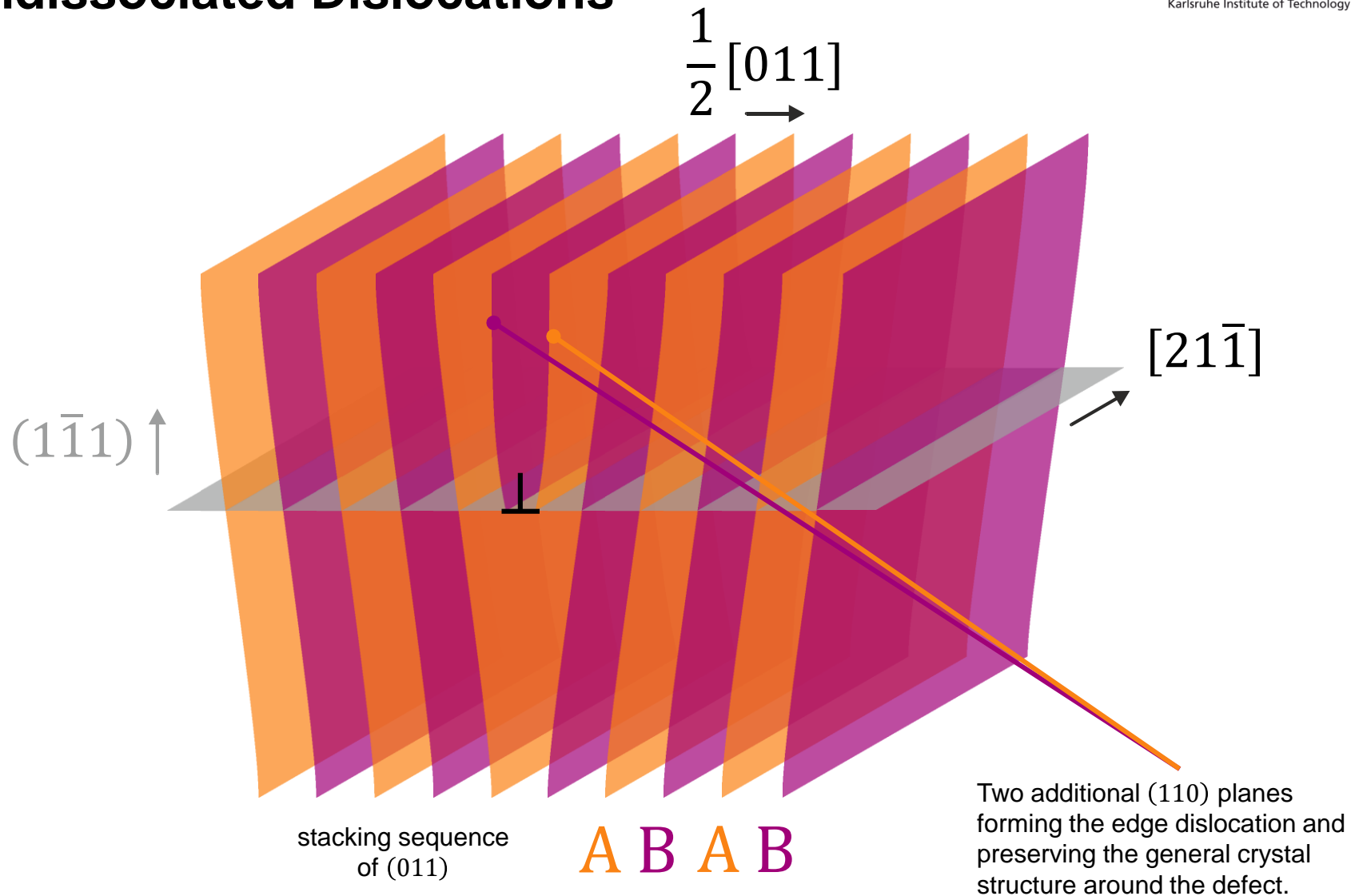


# Undissociated Dislocations

Laue indexing: (220)



# Undissociated Dislocations

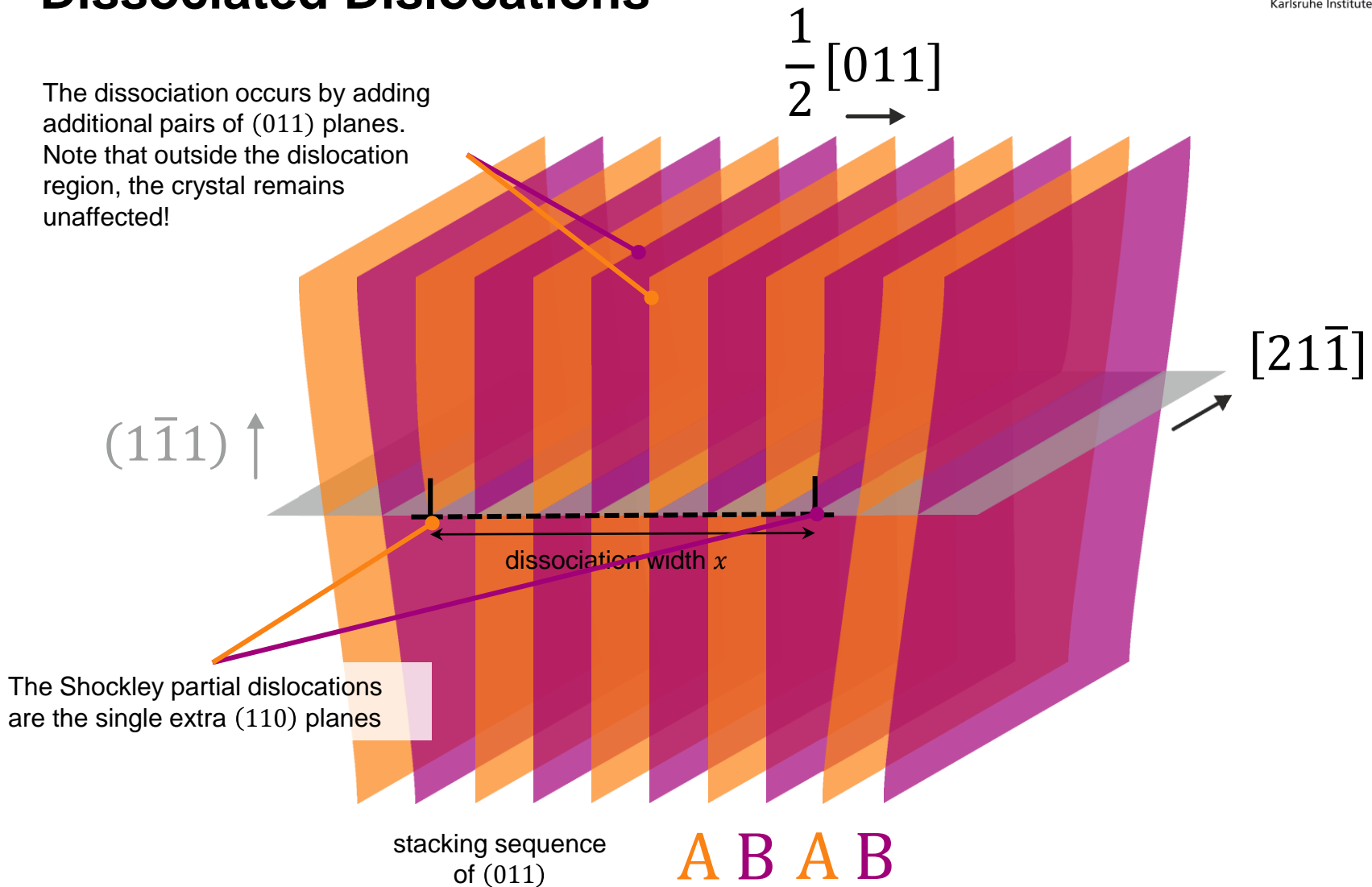


# Shockley Partial Dislocations

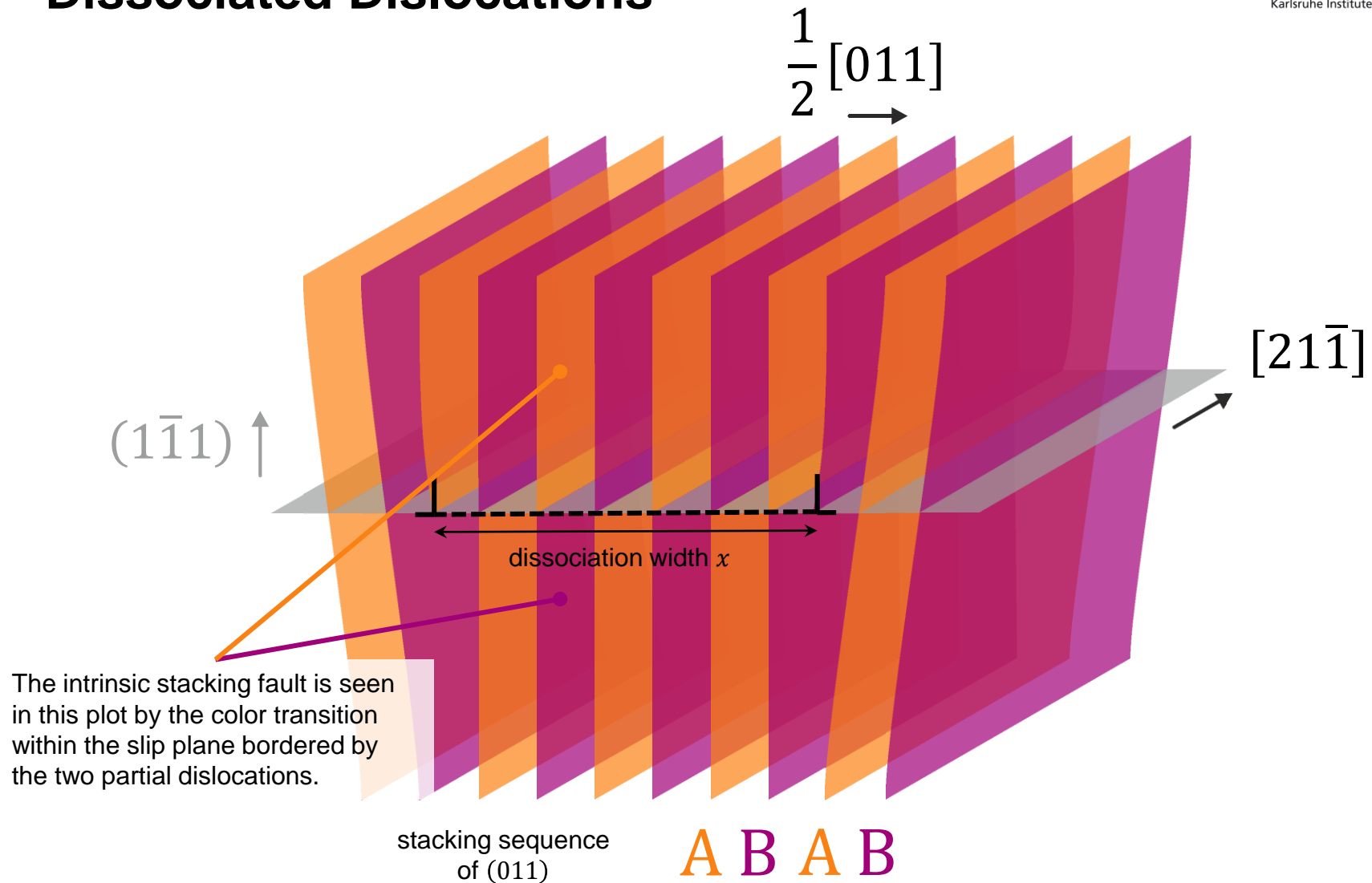
- As we have seen in Ch. 4c, the line energy (as the largest contribution to the dislocation energy) scales with  $\frac{W}{L} \propto G b^2$ .
- Since  $\frac{1}{2}\langle 1\bar{1}0 \rangle$  is the shortest distance between atoms in an A1 crystal structure, any further reduction in Burgers vector length leads to a further distortion of the crystal! The dissociation of dislocations is therefore restricted to special cases.
- One of these cases is the formation of Shockley partial dislocations:
 
$$\frac{1}{2}[011] = \frac{1}{6}[121] + \frac{1}{6}[\bar{1}12]$$
- When neglecting the character of the dislocation and the interaction energy between the partials, we can estimate  $\propto b^2: \frac{1}{2} > \frac{1}{6} + \frac{1}{6} = \frac{1}{3}$ .
- **Shockley partial dislocations border an intrinsic stacking fault.**

# Dissociated Dislocations

The dissociation occurs by adding additional pairs of (011) planes. Note that outside the dislocation region, the crystal remains unaffected!

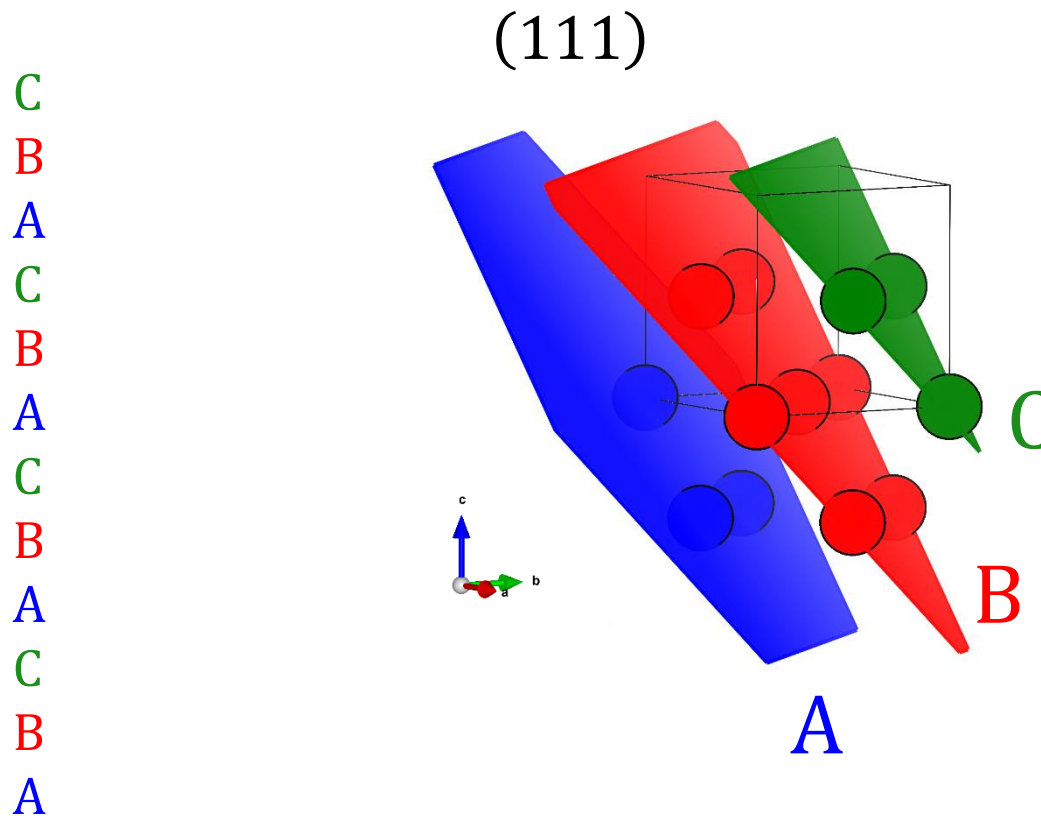


# Dissociated Dislocations



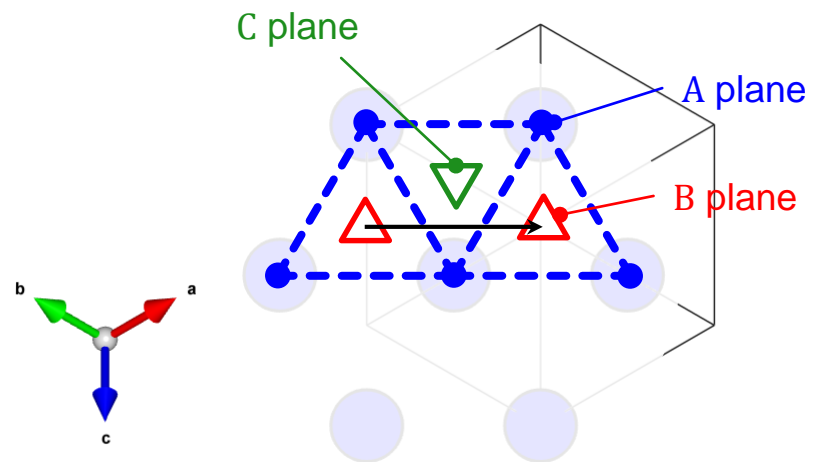
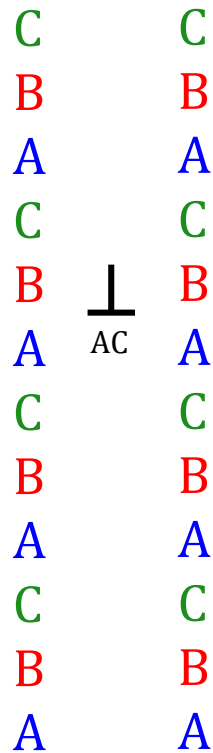
# Shockley Partial Dislocations

- Undistorted stacking sequence in A1 metals and alloys:



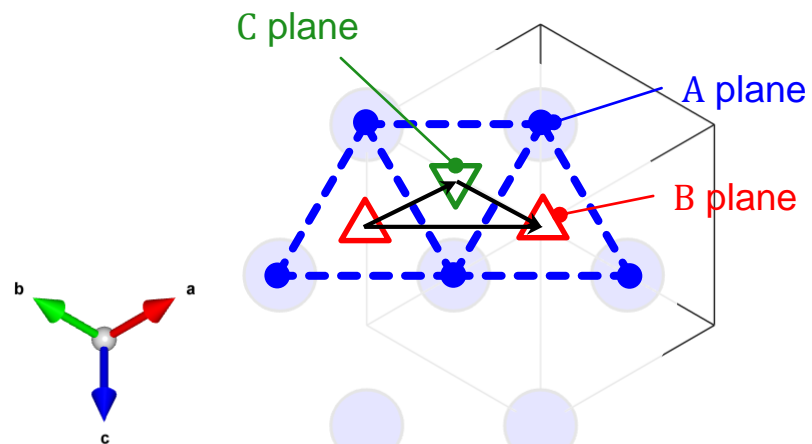
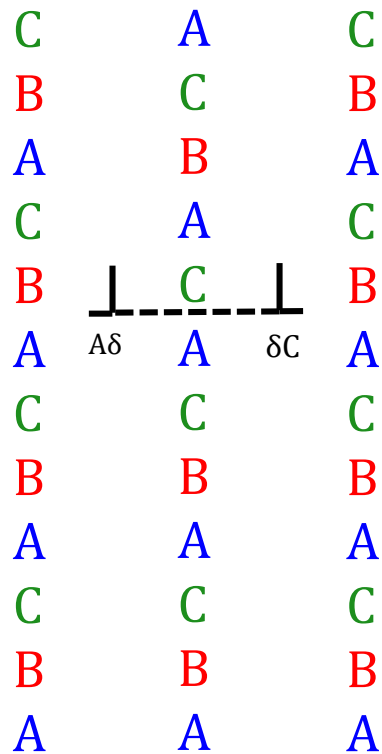
# Shockley Partial Dislocations

- No change for the undissociated dislocation:



# Shockley Partial Dislocations

- In the region bordered by the partial dislocations, an intrinsic stacking fault is formed. The leading partial dislocation opens the stacking fault by shifting from **B** to **C**. The trailing partial closes the stacking fault by shifting from **C** to **B**:



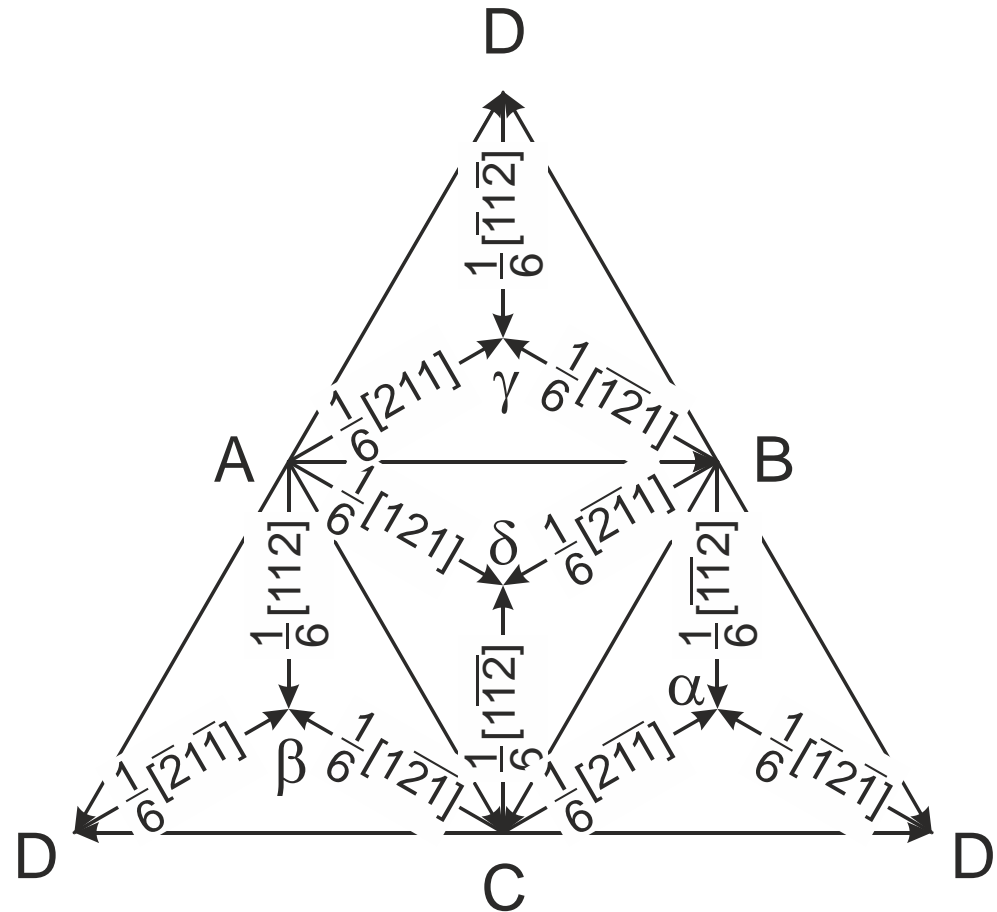


# Thompson Tetrahedron

- Burgers vectors of Shockley partial dislocations are given by connection of the corners with the centers of the slip planes in the Thompson tetrahedron.
- The centers are denoted by Greek lower cases:

$$\frac{1}{2} [011] = \frac{1}{6} [121] + \frac{1}{6} [\bar{1}12]$$

$$AC = A\delta + \delta C$$



# Shockley Partial Dislocations

- The dissociation leads to mostly parallel dislocation character of the two partial and, hence, the dominating interaction of the partials is repelling.
- Due to energy required to form the stacking fault inbetween the partials, an equilibrium dissociation width is achieved:  $\gamma_{\text{iSF}}, [\gamma_{\text{iSF}}] = \frac{mJ}{m^2}$ .
- The stacking fault spans along the dislocation line with the length  $L$  and across the dissociation width  $x$ . The total energy of the intrinsic stacking fault is  $W_{\text{iSF}} = L x \gamma_{\text{iSF}}$ . Specific to the dislocation length:

$$\frac{W_{\text{iSF}}}{L} = x \gamma_{\text{iSF}}$$

- The interaction force between the partials equilibrates this attracting contribution:

$$\frac{F_{\text{iSF}}}{L} = \gamma_{\text{iSF}}$$

# Shockley Partial Dislocations

- Screw components interact with  $\frac{F_x}{L} (y = 0) = \pm \frac{G \cdot b^2}{2\pi} \frac{1}{x}$ . Edge components with  $\frac{F_x}{L} (y = 0) = \pm \frac{G \cdot b^2}{2\pi \cdot (1-\nu)} \frac{1}{x}$ .

- For mixed character, the following equation for the interaction force within the slip plane can be obtained:

$$\frac{F_{\text{dis}}}{L} = \frac{G}{2\pi x} \left( (\mathbf{b}_1 \cdot \mathbf{s})(\mathbf{b}_2 \cdot \mathbf{s}) + \frac{1}{1-\nu} (\mathbf{b}_1 \times \mathbf{s}) \cdot (\mathbf{b}_2 \times \mathbf{s}) \right)$$

- The equilibrium dissociation width is then:

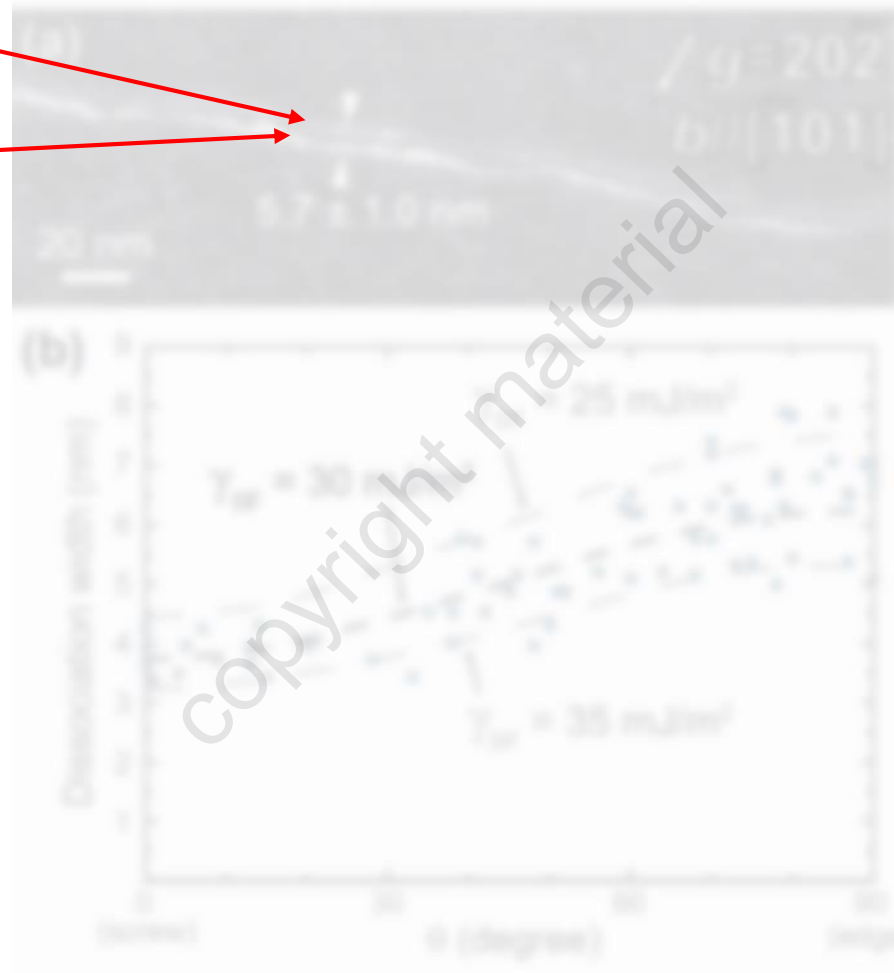
$$x_0 = \frac{G}{2\pi \gamma_{\text{ISF}}} \left( (\mathbf{b}_1 \cdot \mathbf{s})(\mathbf{b}_2 \cdot \mathbf{s}) + \frac{1}{1-\nu} (\mathbf{b}_1 \times \mathbf{s}) \cdot (\mathbf{b}_2 \times \mathbf{s}) \right)$$

- The measurement of equilibrium dissociation width provides direct evidence for the magnitude of the intrinsic stacking fault energy.
- At medium to low stacking fault energies, the dissociation widths are few nanometers only. Only „weak beam dark field“ is possible for imaging.

# Shockley Partial Dislocations

Shockley partial 1

Shockley partial 2



Imaging of a dissociated dislocation in CoCrFeMnNi (A1, Cu structure type) by means of „weak beam dark field“. The dissociation width depends on the character of the full dislocation.

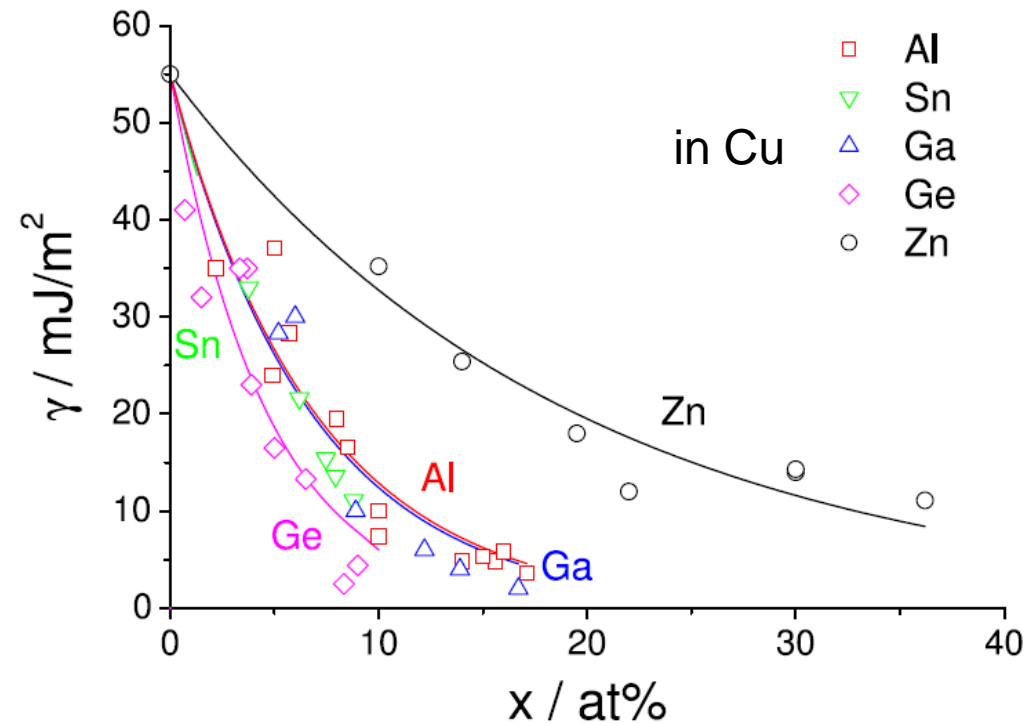
N. Okamoto et al.: “Size effect, critical resolved shear stress, stacking fault energy, and solid solution strengthening in the CrMnFeCoNi high-entropy alloy” in Scientific Reports 6 (2016) 35863

# Dissociated Dislocations

- **Under external force, the pair of Shockley partials behaves like an undissociated dislocation!**
- The **planar dissociation within the slip plane** leads to **very low Peierls** barriers since there are no major displacement components outside the slip plane.
- In contrast to reports in literature, the pair of Shockley partials does only change width under external but **never dissociates or contracts completely**. The latter case can only be achieved when considering relativistic corrections of the interaction force under certain circumstances.

# Intrinsic Stacking Fault Energy $\gamma_{iSF}$

| element | $\gamma_{iSF} / \frac{\text{mJ}}{\text{m}^2}$ |
|---------|---|
| Ag      | 20 ... 30                                     |
| Cu      | 40 ... 60                                     |
| Ni      | ~ 150   |
| Al      | 180 ... 200                                   |



- The stacking fault energy is a key property not only affecting deformation behavior but also recovery and recrystallization.
- Note the relation to the twin boundary energy given in Ch. 3d.

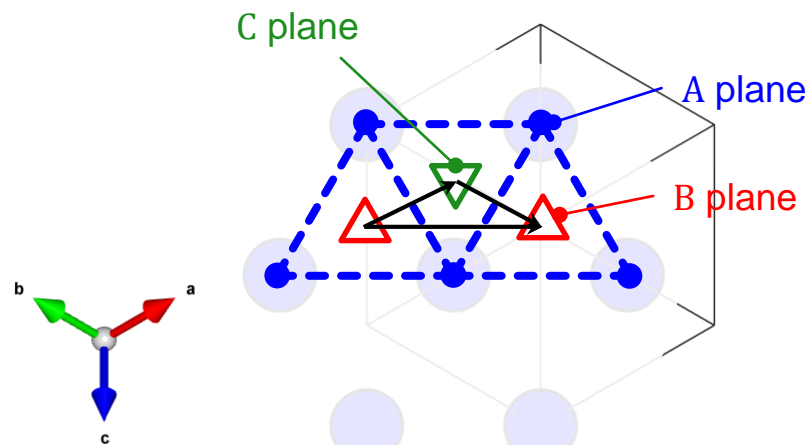
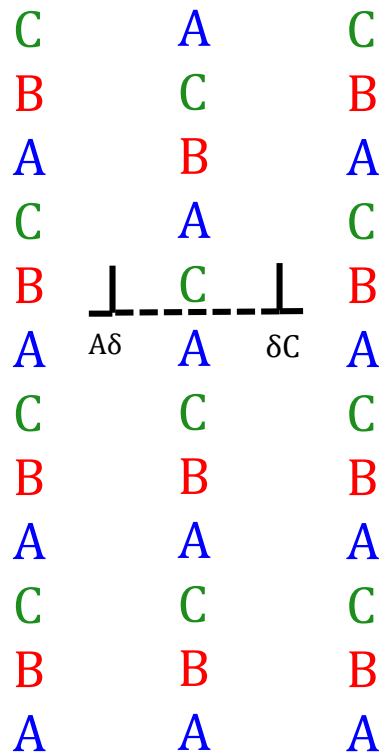
G. Gottstein: "Materialwissenschaft und Werkstofftechnik: Physikalische Grundlagen", Berlin, Heidelberg: Springer Vieweg, Springer-Verlag (2014)  
 J. Freudemberger et al.: "Studies on recrystallization of single-phase copper alloys by resistivity measurements", Acta Materialia 58 (2010) 2324-2329

# Intrinsic Stacking Fault Energy $\gamma_{iSF}$

- The dissociation width controlled by is important when considering cross slip.
- Please see following results:
  - Cu („medium“ stacking fault energy):  
 $G \approx 50 \text{ GPa}$ ,  $b \approx 2.5 \text{ \AA}$ ,  $\gamma_{iSF} \approx 50 \frac{\text{mJ}}{\text{m}^2}$ :  $x_0 \approx 10 \text{ nm}$
  - Al („high“ stacking fault energy):  
 $G \approx 25 \text{ GPa}$ ,  $b \approx 2.9 \text{ \AA}$ ,  $\gamma_{iSF} \approx 190 \frac{\text{mJ}}{\text{m}^2}$ :  $x_0 \approx 1.8 \text{ nm}$

# Attention!

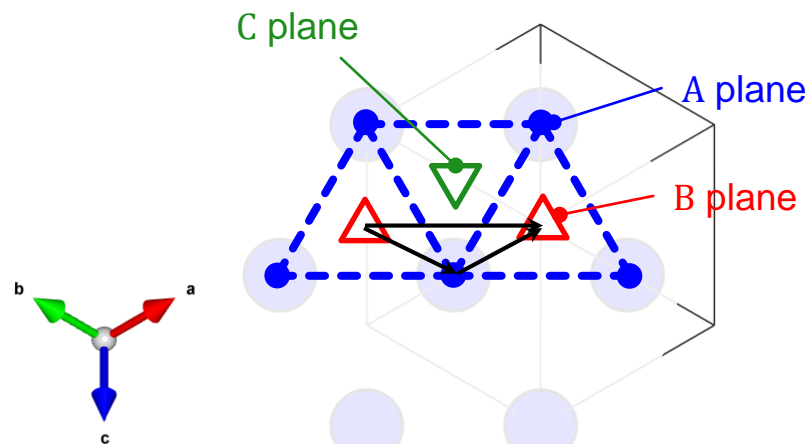
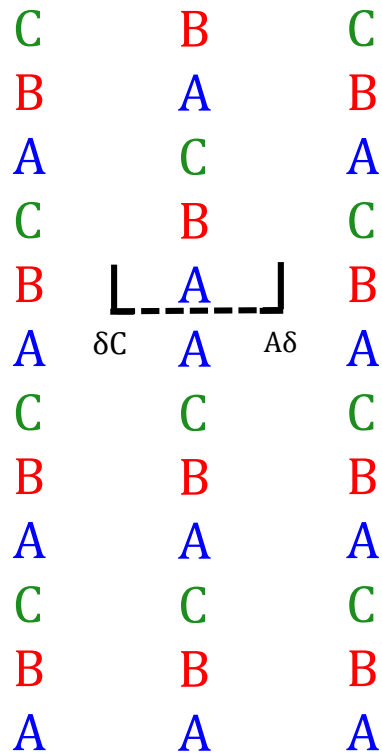
- As mentioned for the Thompson tetrahedron, there is unambiguity if the slip process is not defined. Exchange of leading and trailing partials does not give the same result:  $AC = A\delta + \delta C$  or  $AC = \delta C + A\delta$ !





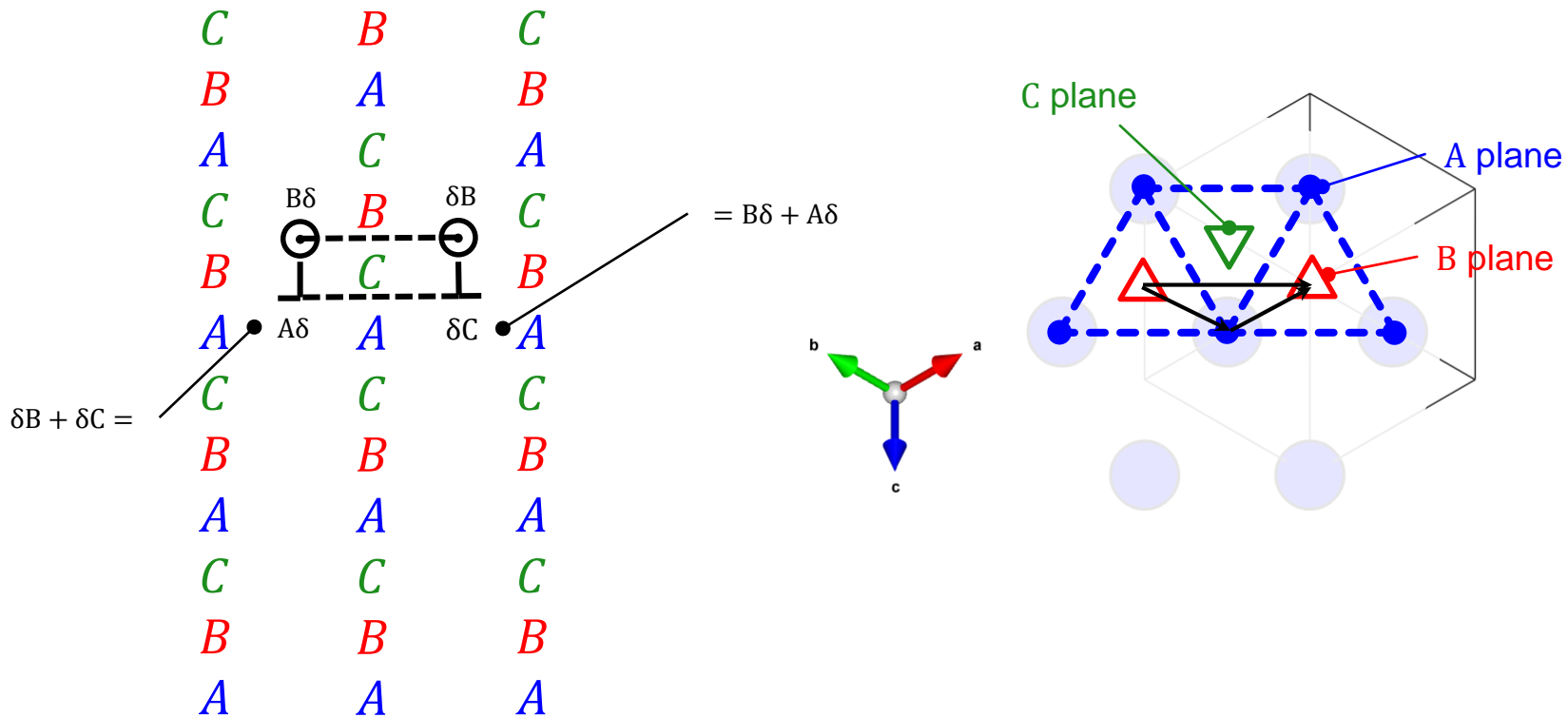
# Attention!

- As mentioned for the Thompson tetrahedron, there is unambiguity if the slip process is not defined. Exchange of leading and trailing partials does not give the same result:  $AC = A\delta + \delta C$  or  $AC = \delta C + A\delta$ !



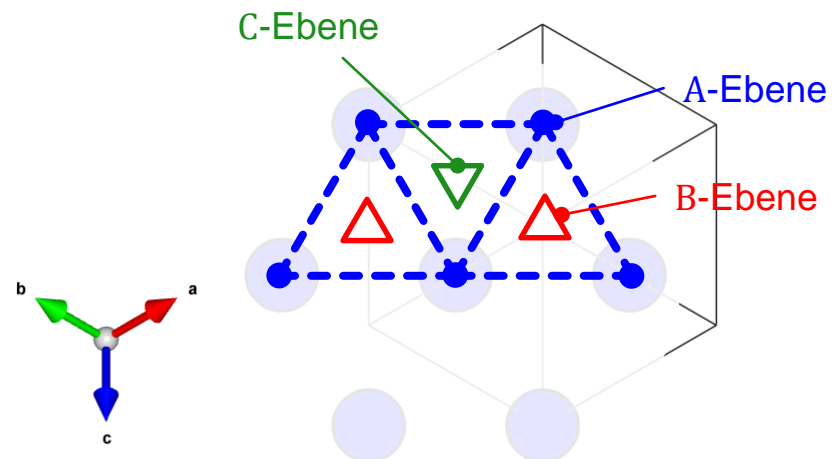
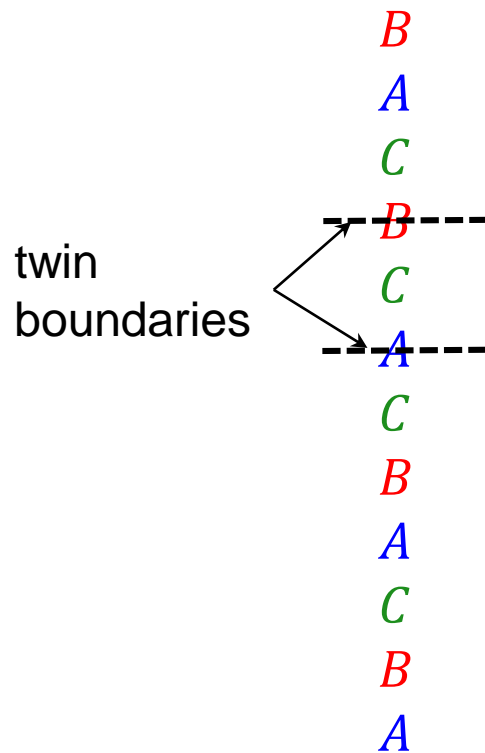
# Attention!

- ...ABCAABCA ... is **not closed packed** and, therefore, **unstable at an tremendous energy!** It will always dissociate into an **extrinsic stacking fault by nucleation of an anti-parallel pair of Shockley partials:**



# Attention!

- The **extrinsic stacking fault** is smallest possible twin lath:



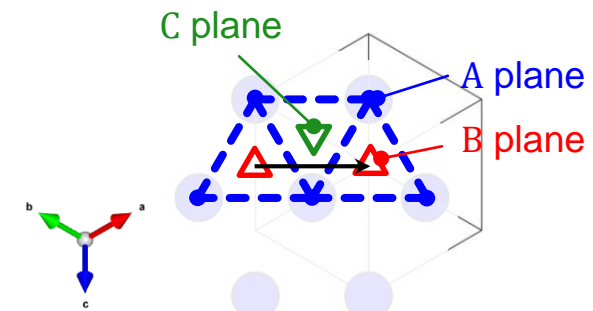
# Generalized Stacking Fault Energy

- With the rise of computational methods, the concept of generalized stacking fault energy became available. From what we have seen in the previous slides, we know:

$\gamma$

A full dislocation with a Burgers vector  $\mathbf{b} = \frac{1}{2}[011]$  (AC) does not change the stacking sequence of the  $\mathbf{n} = (1\bar{1}1)$  (ABC).

The situations before and after displacement have **no excess energy** (ground state: closed packed with perfect stacking sequence).

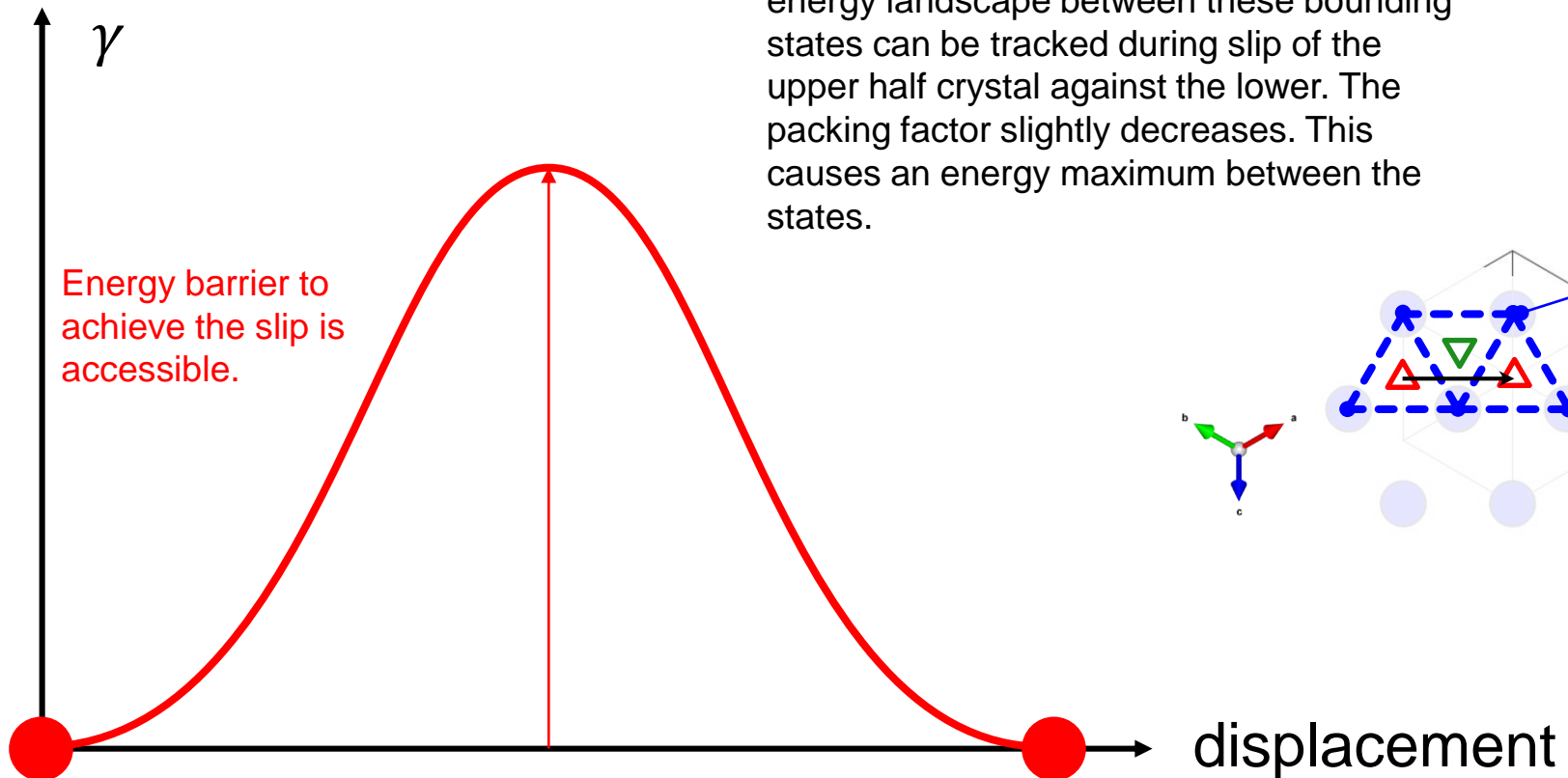


displacement

# Generalized Stacking Fault Energy

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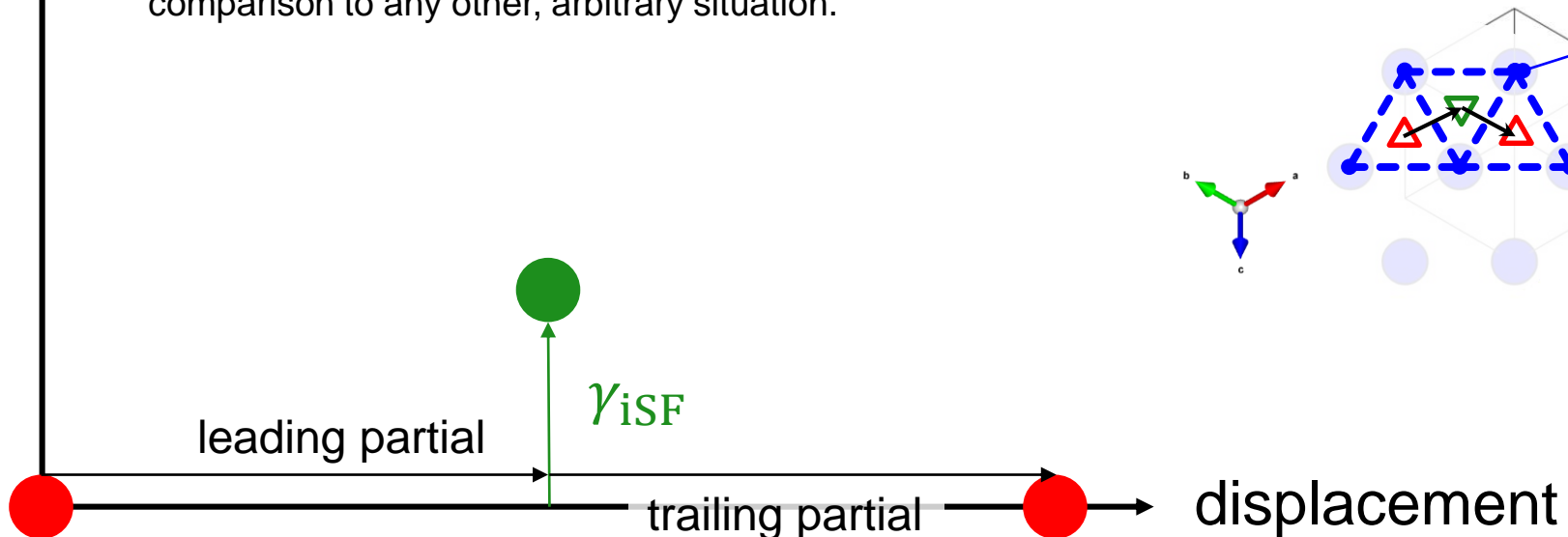
By calculation methods (e.g. MD), the energy landscape between these bounding states can be tracked during slip of the upper half crystal against the lower. The packing factor slightly decreases. This causes an energy maximum between the states.



# Generalized Stacking Fault Energy

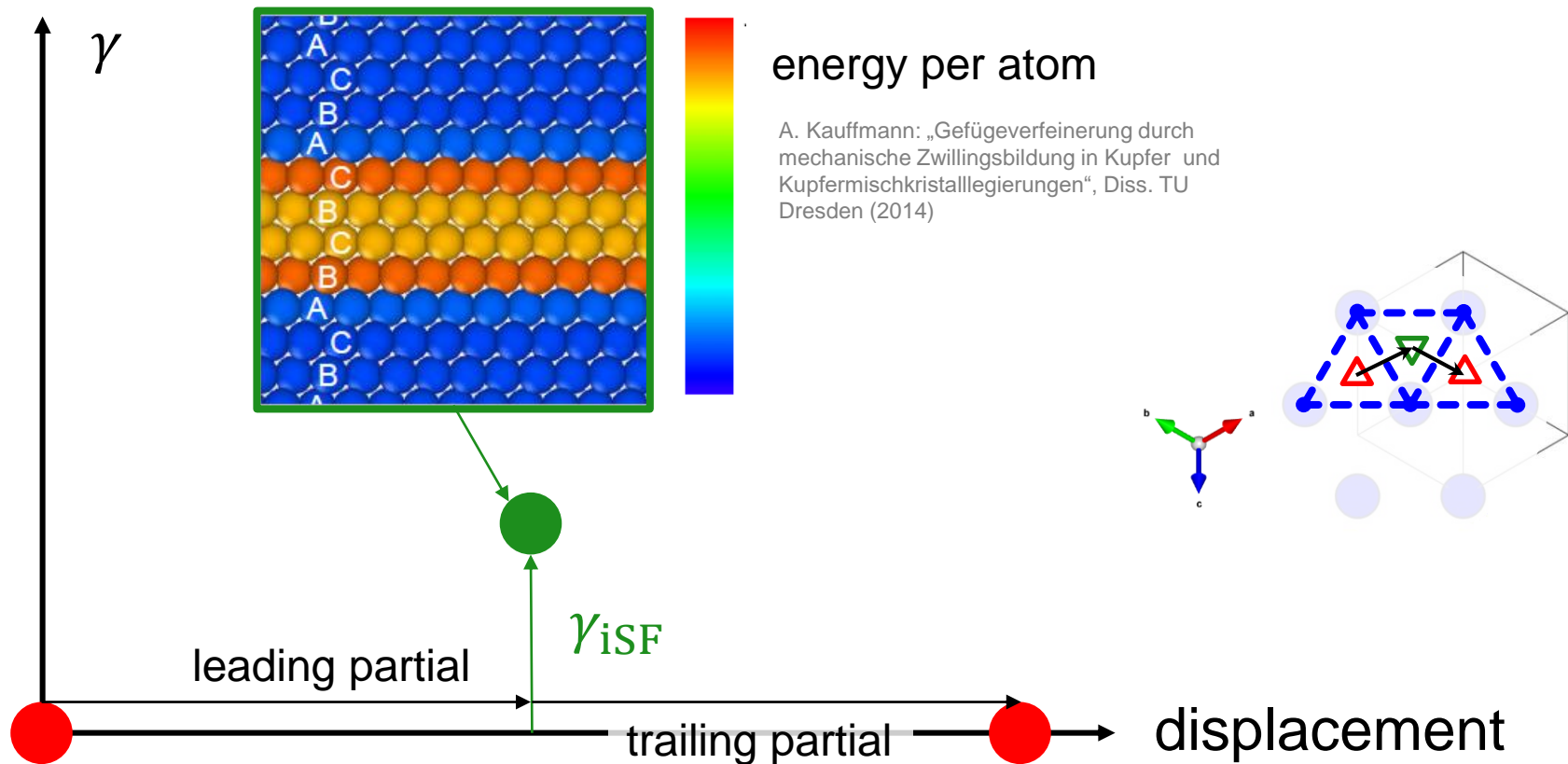
- With the rise of computational methods, the concept of generalized stacking fault energy became available. From what we have seen in the previous slides, we know:

$\gamma$  By the dissociation of the full dislocation, an intrinsic stacking fault is formed. The **intrinsic fault has an higher higher energy  $\gamma_{iSF}$**  than the ground state. Nevertheless, it's still closed packed with maximum coordination (local hcp structure). Therefore, the energy is rather low in comparison to any other, arbitrary situation.



# Generalized Stacking Fault Energy

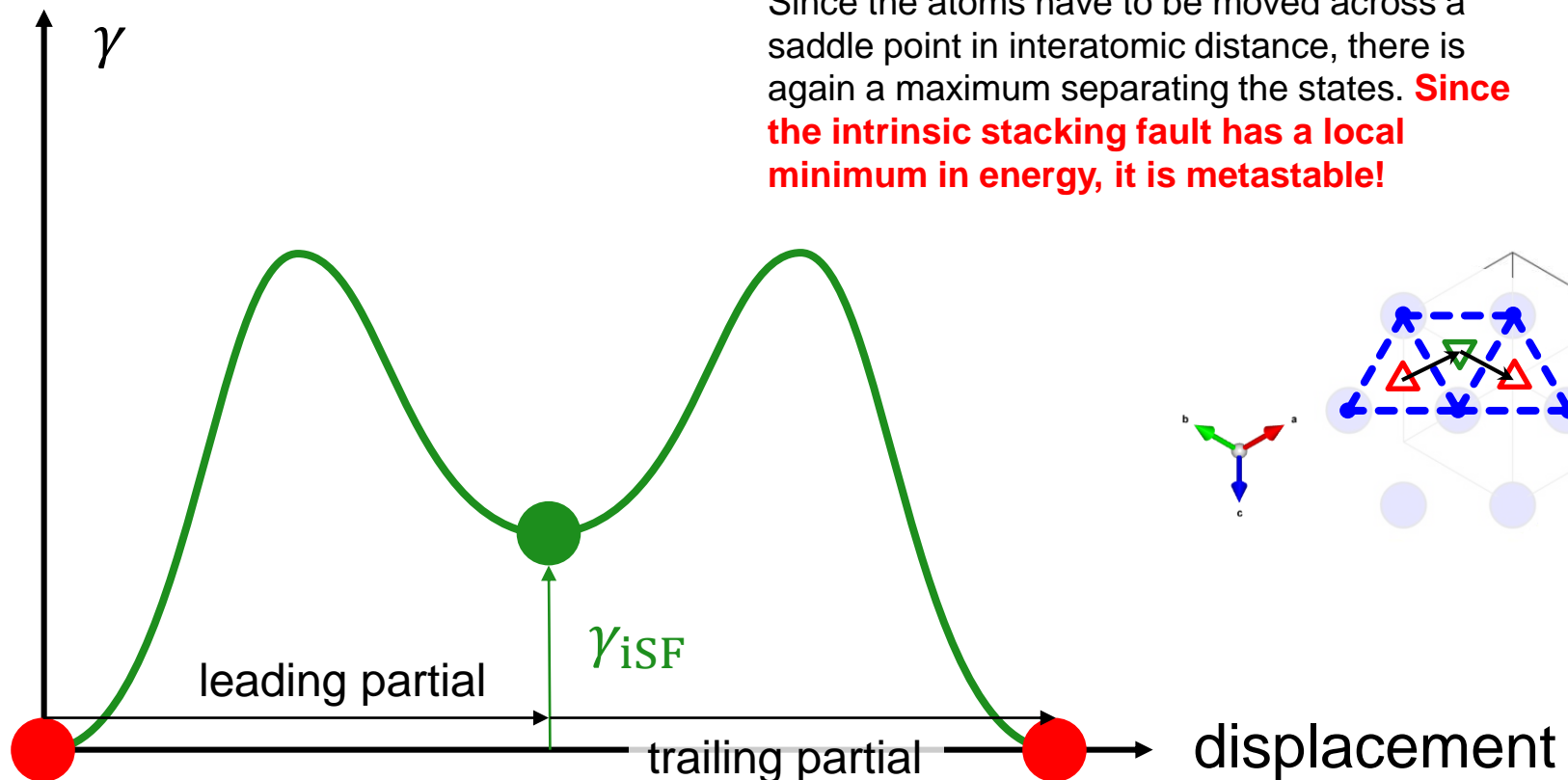
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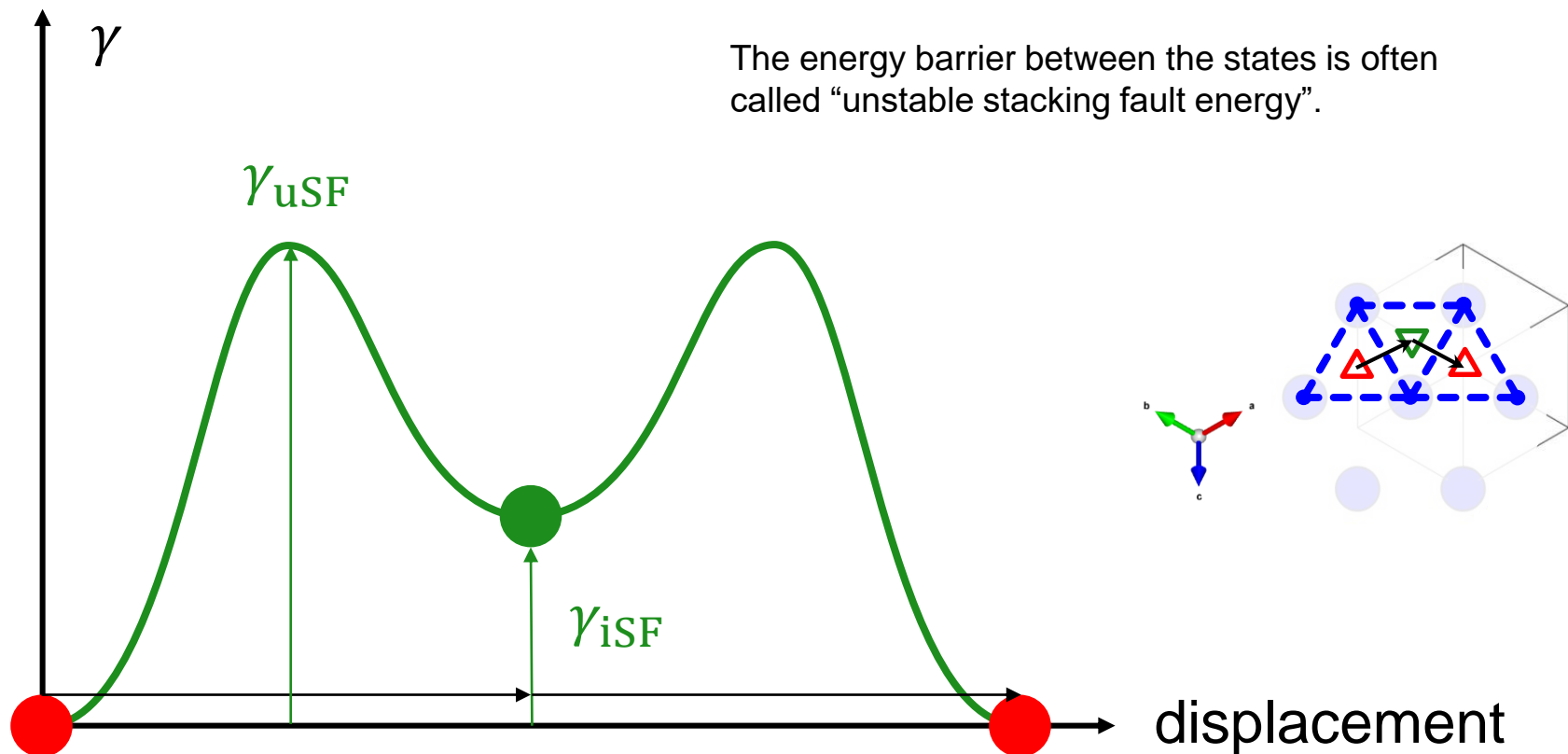
Again the transition states can be computed. Since the atoms have to be moved across a saddle point in interatomic distance, there is again a maximum separating the states. **Since the intrinsic stacking fault has a local minimum in energy, it is metastable!**





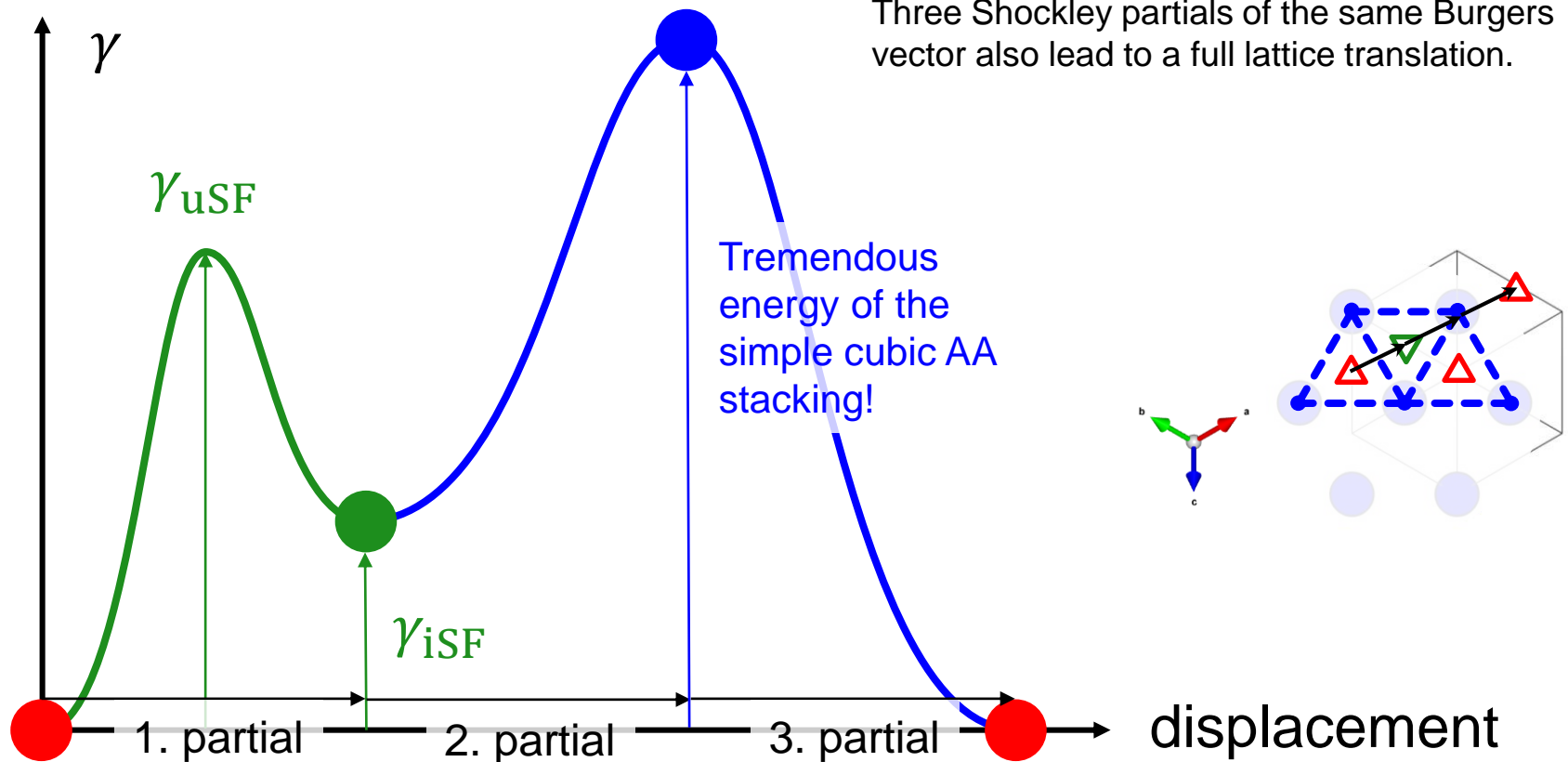
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# Generalized Stacking Fault Energy

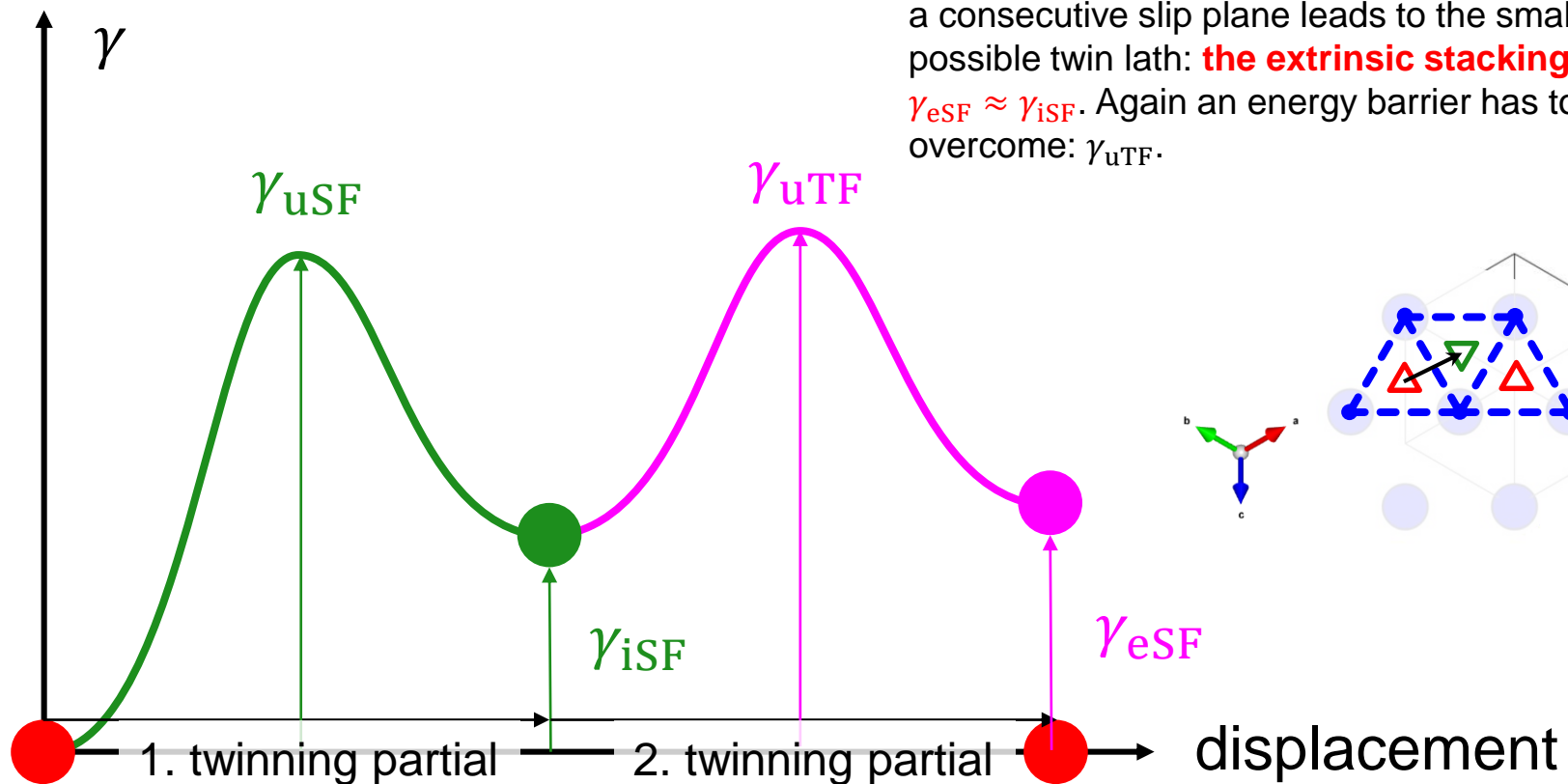
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# Generalized Stacking Fault Energy

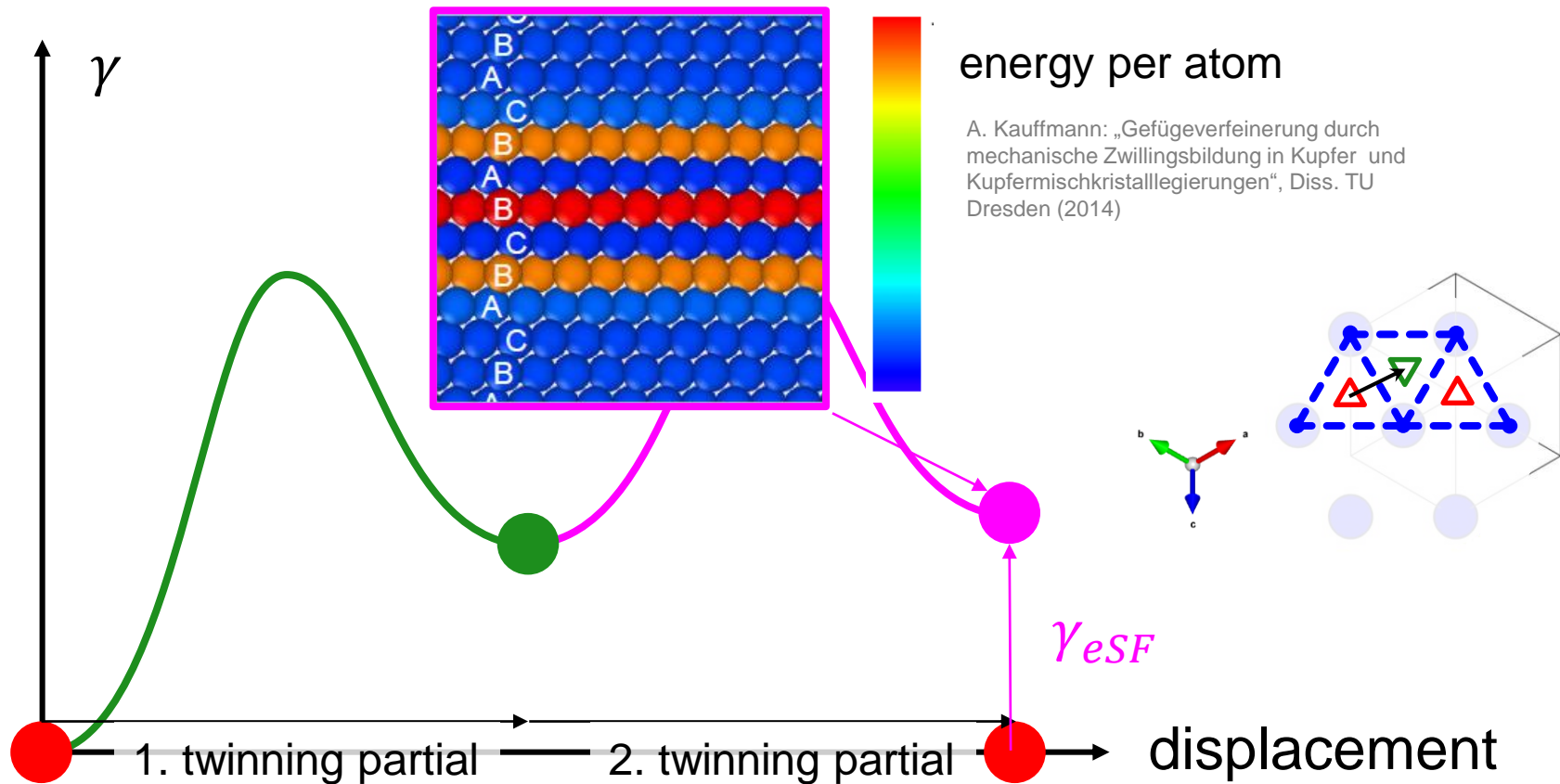
- With the rise of computational methods, the concept of generalized stacking fault energy became available:

The operation of the same partial dislocation on a consecutive slip plane leads to the smallest possible twin lath: **the extrinsic stacking fault**  $\gamma_{eSF} \approx \gamma_{iSF}$ . Again an energy barrier has to be overcome:  $\gamma_{uTF}$ .



# Generalized Stacking Fault Energy

- With the rise of computational methods, the concept of generalized stacking fault energy became available:



# Frank Partial Dislocations

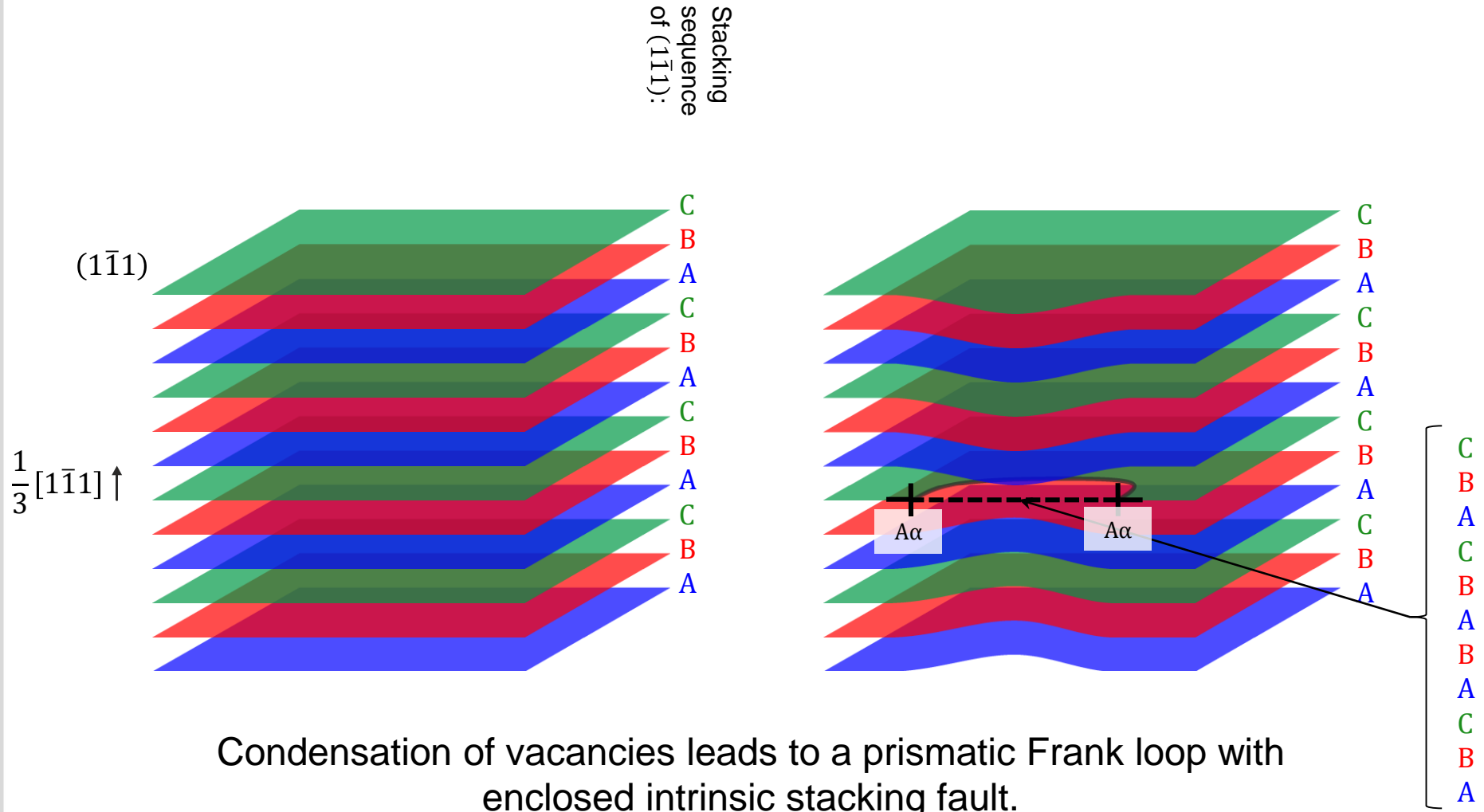
- Another important type of dissociation is achieved by the formation  
**Frank partials:**

$$AC = A\alpha + \alpha C$$

$$\frac{1}{2}[011] = \frac{1}{3}[111] + \frac{1}{6}[\bar{2}11]$$

- Note that the **Burgers vector of Frank partial dislocations exactly bridges the distance between the slip planes of the octahedral slip system** (capital Latin letter with matching Greek lowercase on the opposite tetrahedron face). Therefore, they play an important role in condensation of vacancies and deformation twinning by source mechanisms.
- Frank partial dislocations are considered **sessile!**
- Pure Frank dislocations are formed by condensation of vacancies to negative prismatic loops.

# Frank Partial Dislocations



Condensation of vacancies leads to a prismatic Frank loop with enclosed intrinsic stacking fault.

# Frank Partial Dislocations



Typical fringe contrast by the stacking fault in a prismatic loop in quenched AlMg3. After recovery, the stacking fault is gone and a full dislocation loop has formed. The segments are parallel to  $\langle 1\bar{1}0 \rangle$  within  $\{111\}$ .

Further analysis actually shows that Frank loops are not composed of single Frank partial dislocations but from typically two or three partials very close to each other (either coplanar or metastable stacked).

D. Hull, D. J. Bacon: "Introduction to Dislocations", Amsterdam, etc.: Elsevier (2011)

# Cross Slip

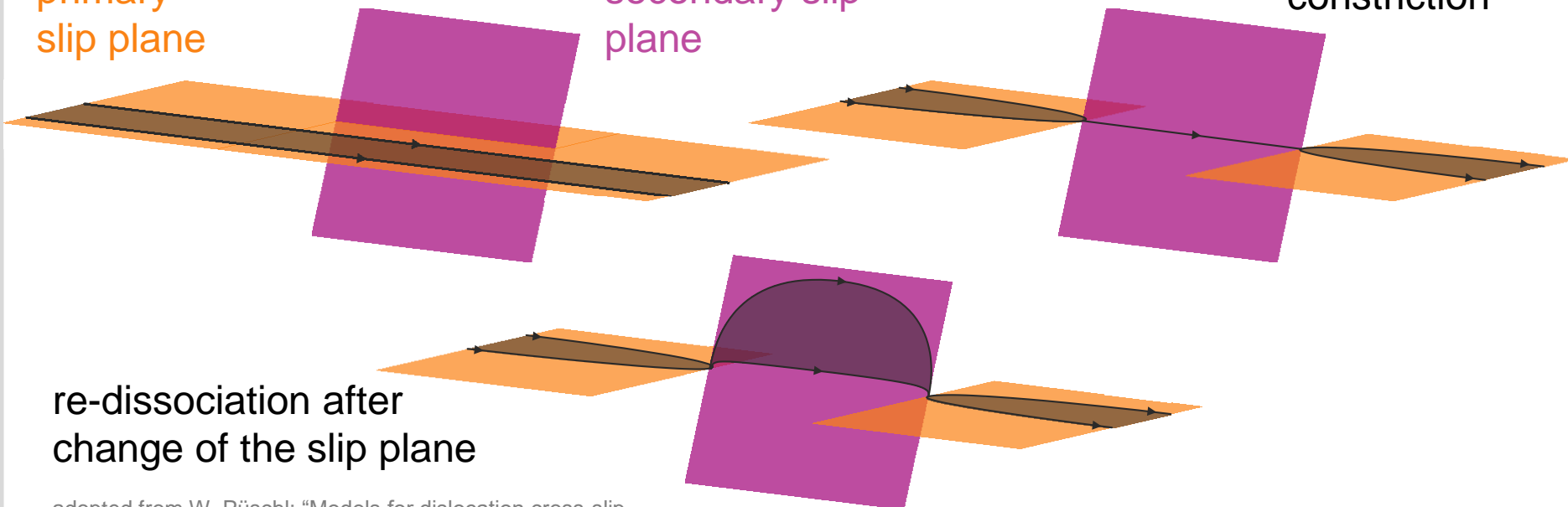
**Friedel-Escaig:** the partials first have to constrict in the intersection of the slip planes to a full screw dislocation in order to change the slip plane. This is considered as the major cross slip mechanism in A1 metals and alloys. The constriction can be assisted by thermal fluctuations and the process is hence thermally activated.

primary  
slip plane

secondary slip  
plane

constriction

re-dissociation after  
change of the slip plane

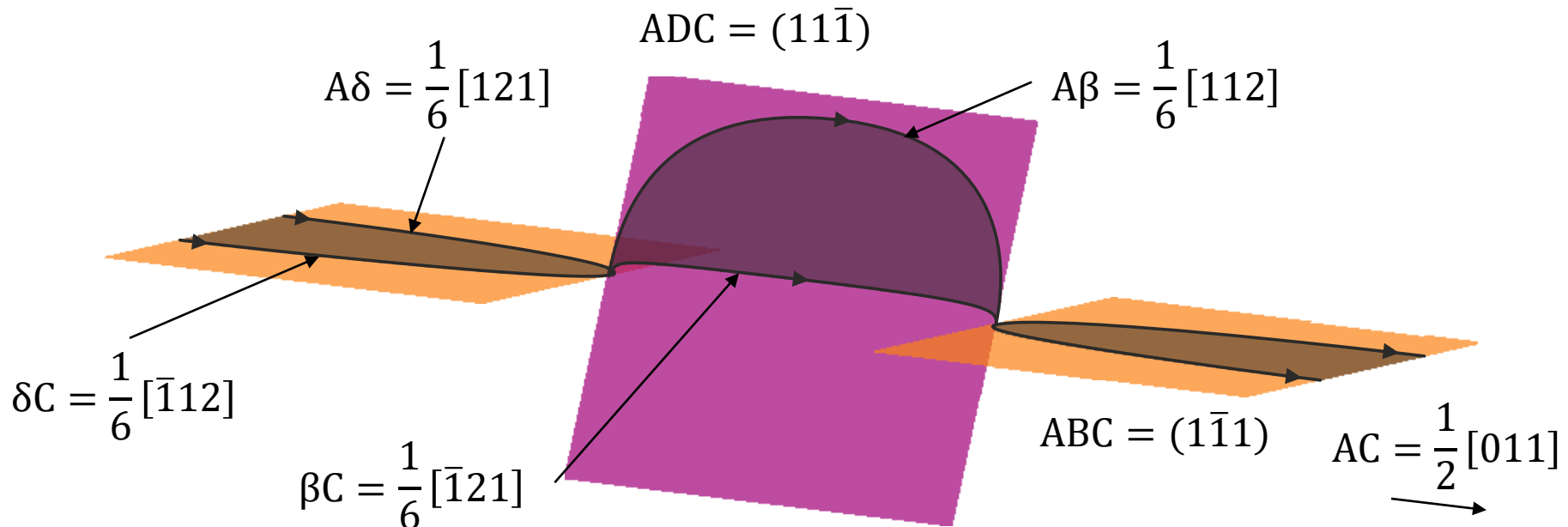


adopted from W. Püschl: "Models for dislocation cross-slip in close-packed crystal structures: a critical review" in Progress in Materials Science 47 (2002) 415–461



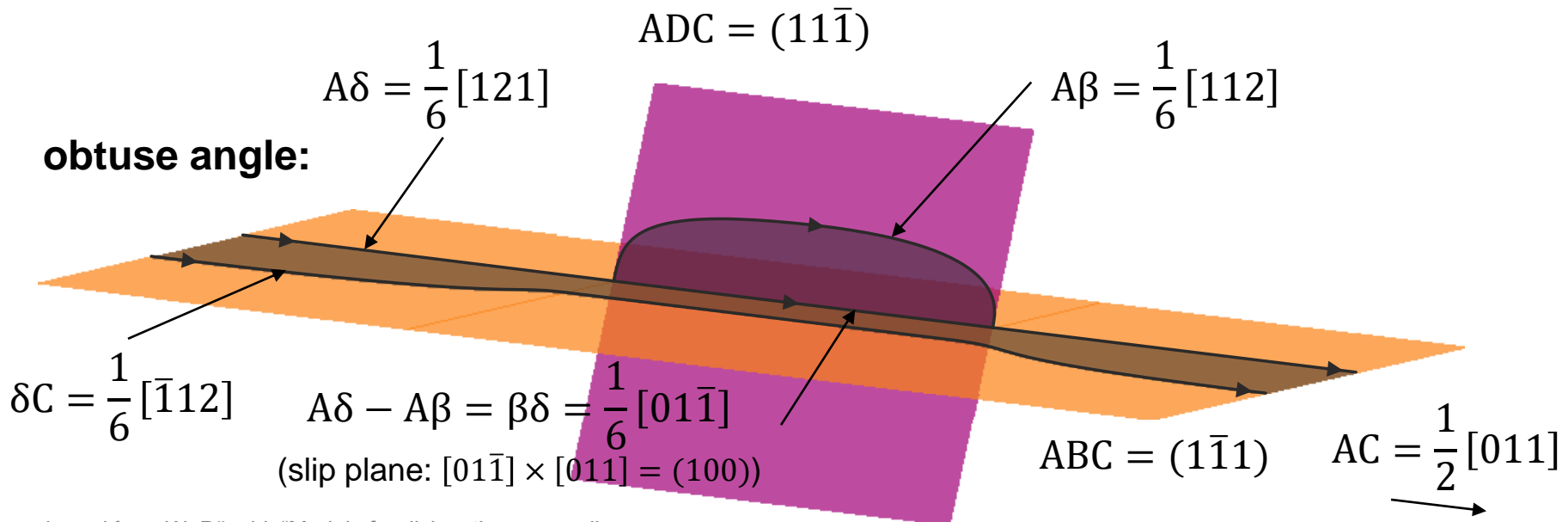
# Cross Slip

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# Cross Slip

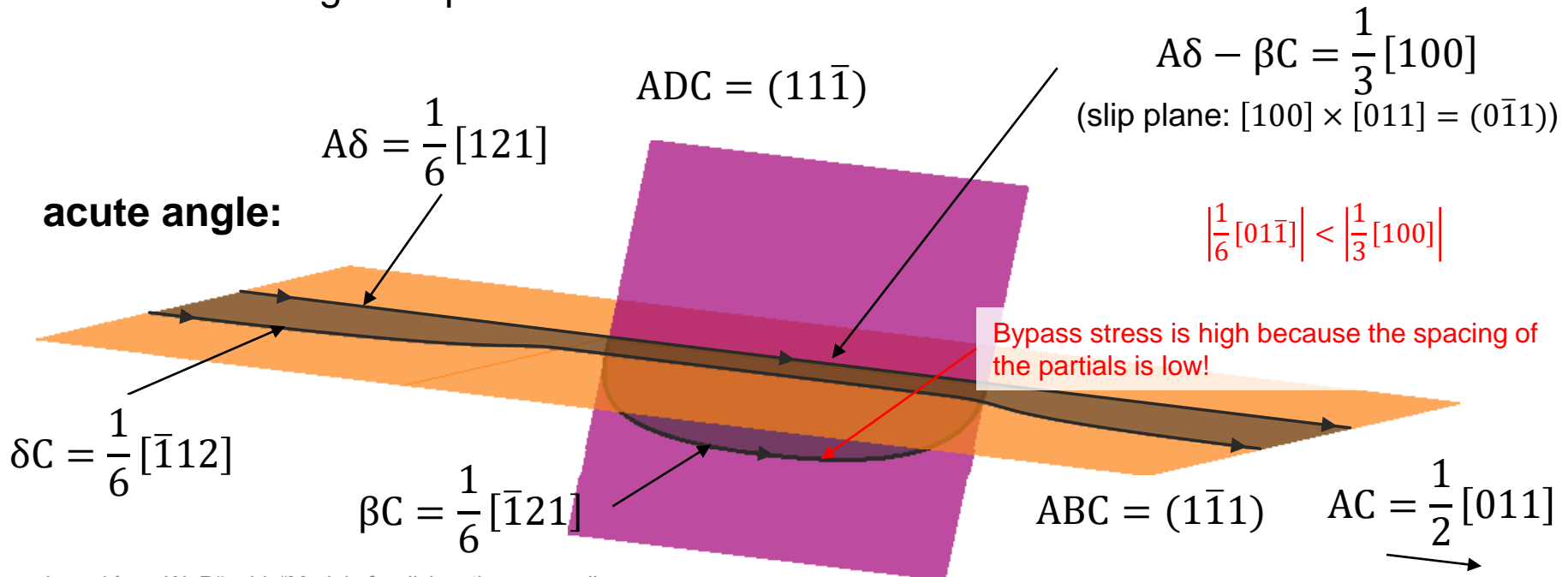
**Fleischer:** the stacking fault changes the slip plane at once! Due to the different Burgers vector of the leading partial in the secondary slip plane, there must be a new segment in the intersection of the slip planes mediating the difference. The segment has  $\frac{1}{6}[01\bar{1}]$  on  $(100)$  and is sessile! The process is maybe active at high stresses and high temperatures.



adopted from W. Püschl: "Models for dislocation cross-slip in close-packed crystal structures: a critical review" in Progress in Materials Science 47 (2002) 415–461

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adopted from W. Püschl: "Models for dislocation cross-slip in close-packed crystal structures: a critical review" in Progress in Materials Science 47 (2002) 415–461

# Cross Slip

- **Cross slip is a vital contribution to static and dynamic recovery.** It **allows** dislocations to leave the slip plane and **annihilate with dislocations of same sign** or **form a metastable pattern with dislocations of same sign.**
- **Both fundamental processes are assisted by thermal fluctuation.** In order to suppress cross slip, the temperature of deformation can be decreased. Hence, (dynamic) recovery can be reduced by this as well and higher stress levels are achieved by dislocation strengthening.
- **Increasing dissociation width significantly decreases probability for cross slip.** This can be achieved by lowering stacking fault energy.

# Dislocation Reactions

- In Ch. 4d, we introduced **dislocation bypass** and **dislocation intersection** as important contributions to dislocation strengthening and work-hardening.
- In real crystal structures, there are **additional interaction** possibilities due to the **discrete nature of the crystal (finite number of slip system and slip planes with various slip directions)**, namely the **reaction of parallel dislocations on inclined slip planes**.
- The **probability** for such reactions is again assessed on the basis of the introduced concepts:
  - **Line energy**: in case the Burgers vector of the reaction is significantly shorter than the Burgers vector of the original dislocations, the reaction becomes energetically feasible.
  - **Interaction stress**: in case the interaction stress of the initial dislocations is not too high for the applied stress, the reaction of the dislocation segments is possible.

# Dislocation Reactions

## ■ Dislocation reactions **on the same slip plane**:

### ■ **Annihilation**:

- Slip planes of the two dislocations:  $\mathbf{n}_1 = \mathbf{n}_2 = (111)$
- Burgers vectors of the initial dislocations:  $\mathbf{b}_1 = -\mathbf{b}_2 = \frac{1}{2}[\bar{1}10]$
- Burgers vector of the reaction product: no net Burgers vector

### ■ **Recombination** to the third Burgers vector within the slip plane:

- Slip planes of the two dislocations:  $\mathbf{n}_1 = \mathbf{n}_2 = (111)$
- Burgers vectors of the initial dislocations:  
 $\mathbf{b}_1 = \frac{1}{2}[\bar{1}10]$  und  $\mathbf{b}_2 = \frac{1}{2}[10\bar{1}]$
- Burgers vector of the reaction product:  $\frac{1}{2}[\bar{1}10] + \frac{1}{2}[10\bar{1}] = \frac{1}{2}[01\bar{1}]$

**There are two initial full dislocations which recombine to a single full dislocation!**

- **Any other reaction leads to a much longer Burgers vector of the reaction product and is, therefore, not feasible.**

# Dislocation Reactions

## ■ Dislocation reactions **on different slip planes:**

### ■ **Recombination** to another dislocation of the octahedral slip systems:

- Slip planes of the two dislocations:  $\mathbf{n}_1 = (111)$  and  $\mathbf{n}_2 = (1\bar{1}1)$

- Burgers vectors of the initial dislocations:

$$\mathbf{b}_1 = \frac{1}{2}[\bar{1}10] \text{ and } \mathbf{b}_2 = \frac{1}{2}[10\bar{1}]$$

- Burgers vector of the reaction product:  $\mathbf{b} = \frac{1}{2}[\bar{1}10] + \frac{1}{2}[10\bar{1}] = \frac{1}{2}[01\bar{1}]$

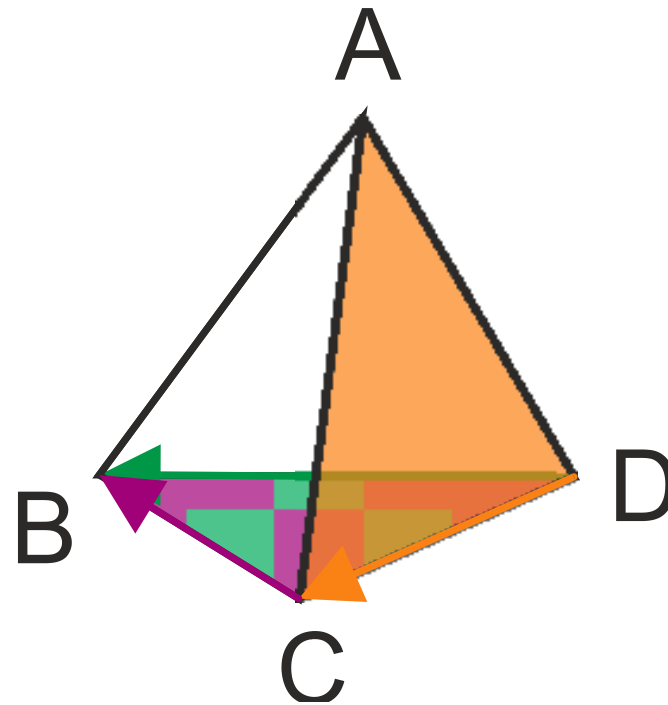
**There are two initial full dislocations which recombine to a single full dislocation!**

- Dislocation line of the reaction product:  $\mathbf{s} = (111) \times (1\bar{1}1) = [10\bar{1}]$

- Slip plane of the reaction product:  $\mathbf{n} = \mathbf{s} \times \mathbf{b} = [10\bar{1}] \times \frac{1}{2}[01\bar{1}] = (111)$

**The new dislocation is glissile** since it is a dislocation on an octahedral slip system  $(111)\frac{1}{2}[01\bar{1}]$ .

# Dislocation Reactions



- and ■ are the initial dislocations
- is the reaction product



# Dislocation Reactions

## ■ Dislocation reactions **on different slip planes:**

### ■ **Lomer-Lock:**

■ Slip planes of the two dislocations:  $\mathbf{n}_1 = (111)$  and  $\mathbf{n}_2 = (\bar{1}\bar{1}1)$

■ Burgers vectors of the initial dislocations:

$$\mathbf{b}_1 = \frac{1}{2}[\bar{1}10] \text{ and } \mathbf{b}_2 = \frac{1}{2}[101]$$

■ Burgers vector of the reaction product:  $\mathbf{b} = \frac{1}{2}[\bar{1}10] + \frac{1}{2}[101] = \frac{1}{2}[011]$

**There are two initial full dislocations which recombine to a single full dislocation!**

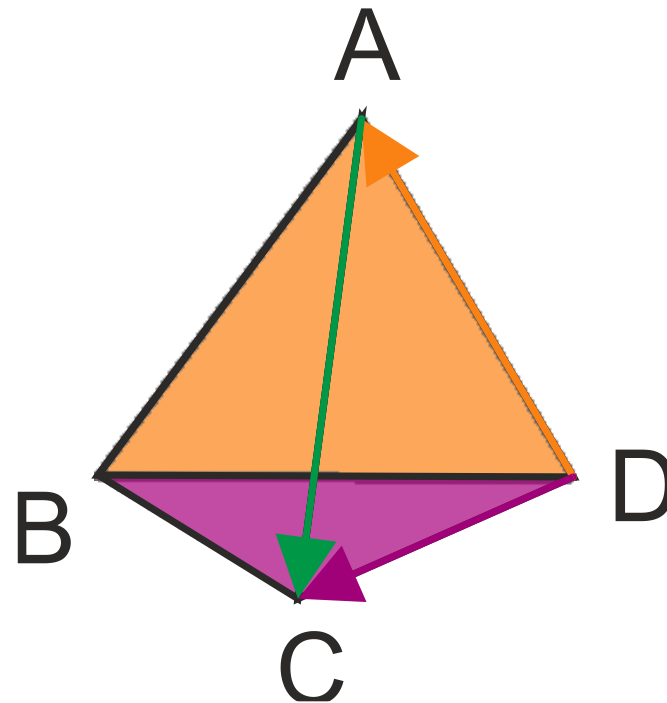
■ Dislocation line of the reaction product:  $\mathbf{s} = (111) \times (\bar{1}\bar{1}1) = [0\bar{1}1]$

■ Slip plane of the reaction product:  $\mathbf{n} = \mathbf{s} \times \mathbf{b} = [0\bar{1}1] \times \frac{1}{2}[011] = (100)$

The  $\{100\}$  do not belong to the octahedral slip systems. **The reaction product is sessile: lock.** In literature, it's usually referred to as „stair rod“.

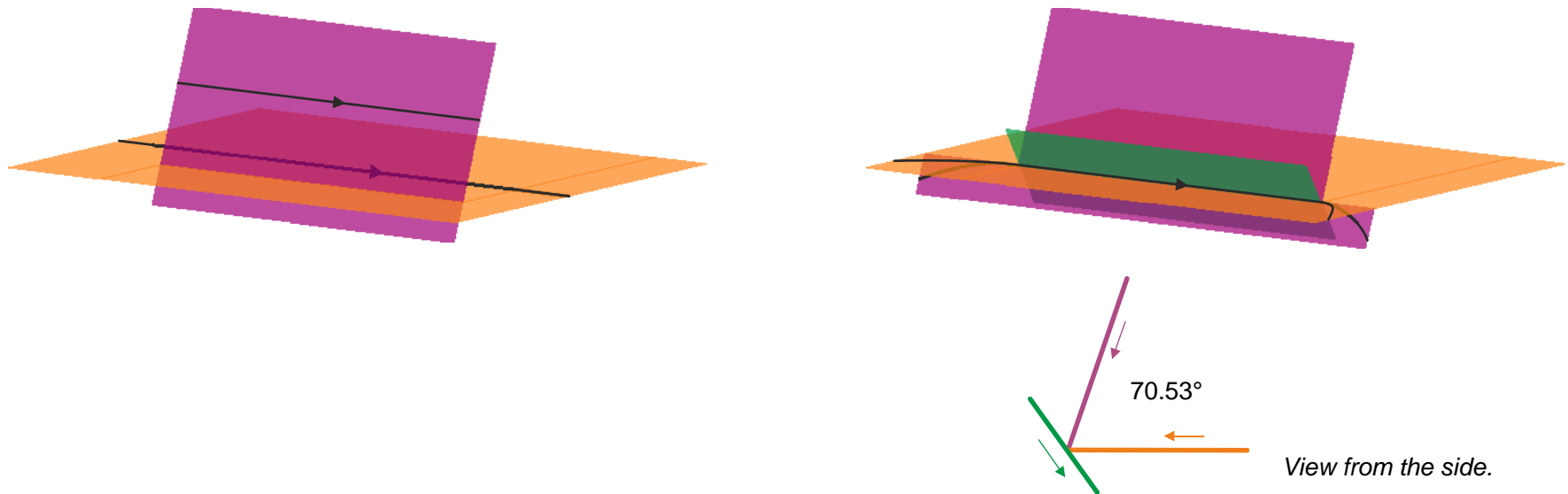
■ **Any other reaction leads to a much longer Burgers vector of the reaction product and is, therefore, not feasible.**

# Dislocation Reactions



- and ■ are the initial dislocations
- is the reaction product (the slip plane is not shown)

# Dislocation Reactions



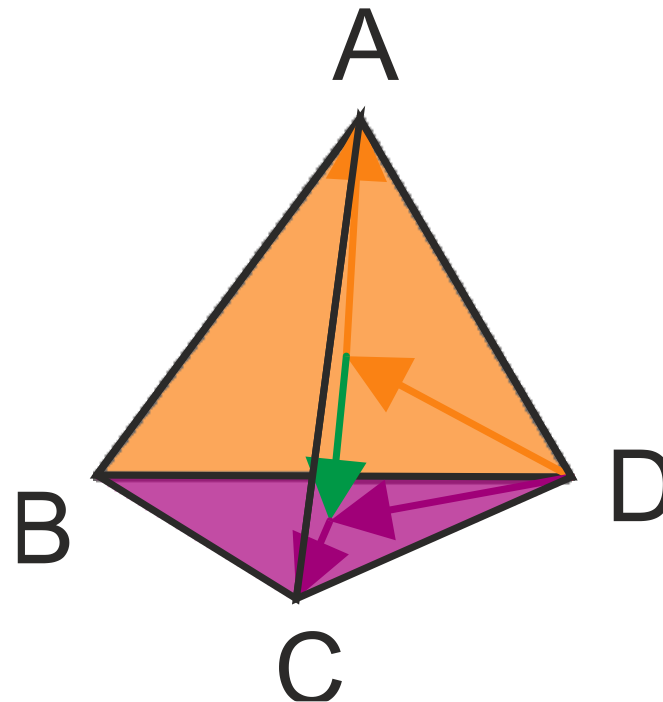
- and ■ are the initial dislocations
- is the reaction product

**The sessile segment acts as obstacle for the dislocation motion on the two slip planes. In case of an operating dislocation source on either of the slip planes, pile-ups are created. The glissile segments can form glide sources.**

# Dislocation Reactions

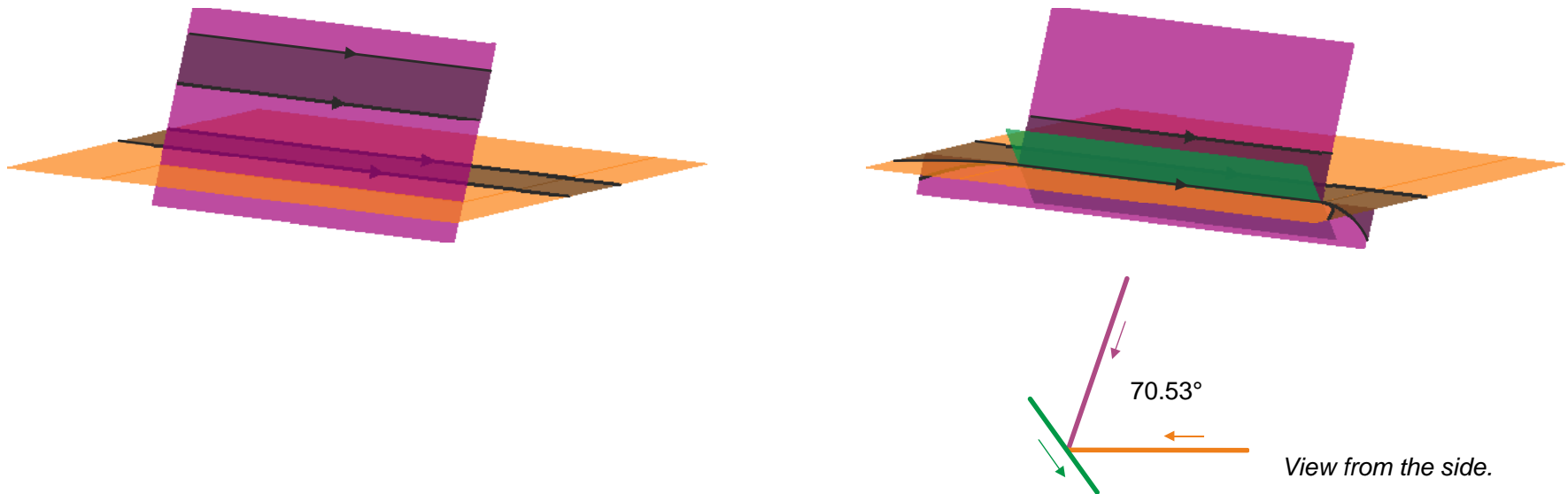
- Dislocation reactions **on different slip planes, but considering the dissociation of the dislocations:**
  - **Lomer-Cottrell-Lock:**
    - Slip planes of the two dislocations:  $\mathbf{n}_1 = (111)$  und  $\mathbf{n}_2 = (\bar{1}\bar{1}1)$
    - Burgers vectors of the initial dislocations:  
 $\mathbf{b}_1 = \frac{1}{6}[\bar{1}2\bar{1}] + \frac{1}{6}[\bar{2}11]$  and  $\mathbf{b}_2 = \frac{1}{6}[1\bar{1}2] + \frac{1}{6}[211]$
    - Burgers vector of the reaction product  $\mathbf{b} = \frac{1}{6}[\bar{1}2\bar{1}] + \frac{1}{6}[1\bar{1}2] = \frac{1}{6}[011]$   
**Two Shockley partial dislocations react to a single Lomer-Cottrell lock with much shorter Burgers vector!**
    - Dislocation line of the reaction product:  $\mathbf{s} = (111) \times (\bar{1}\bar{1}1) = [0\bar{1}1]$
    - Slip plane of the reaction product:  $\mathbf{n} = \mathbf{s} \times \mathbf{b} = [0\bar{1}1] \times \frac{1}{6}[011] = (100)$   
 The  $\{100\}$  do not belong to the octahedral slip systems. **The reaction product is sessile: lock.** In literature, it's usually referred to as „stair rod“.
  - **Any other reaction leads to a much longer Burgers vector of the reaction product and is, therefore, not feasible.**

# Dislocation Reactions



- and ■ are the initial dislocations
- is the reaction product (the slip plane is not shown)

# Dislocation Reactions



- and ■ are the initial dislocations
- is the reaction product

**The sessile segment acts as obstacle for the dislocation motion on the two slip planes. In case of an operating dislocation source on either of the slip planes, pile-ups are created. The glissile segments can form glide sources.**

# Summary

- In A1 metals and alloys, closed packed planes and closed packed directions act as slip systems: **octahedral slip systems**.
- **Depending on the intrinsic stacking fault energy, dislocations are dissociated.** The dissociation **restricts** the **cross slip probability** of screw dislocations and, therefore, the **ability to dynamically recover**.
- The reaction of dislocations on different slip planes can lead to the **formation of locks**. **Locks cause pile-up of dislocations and formation of glide sources**. Hence, locks play a vital role in work-hardening of A1 metals and alloys.