KIT
Karlsruhe Institute of Technology

IAM
Institute for Applied Materials

Plasticity

Lecture for “Mechanical Engineering” and “Materials Science and Engineering”
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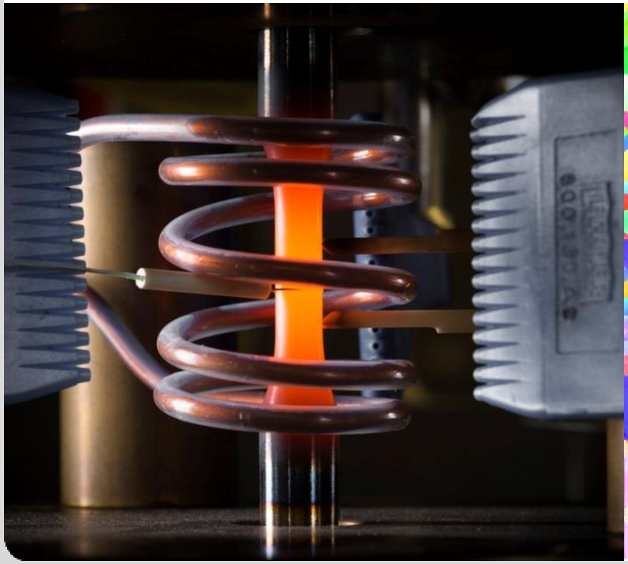
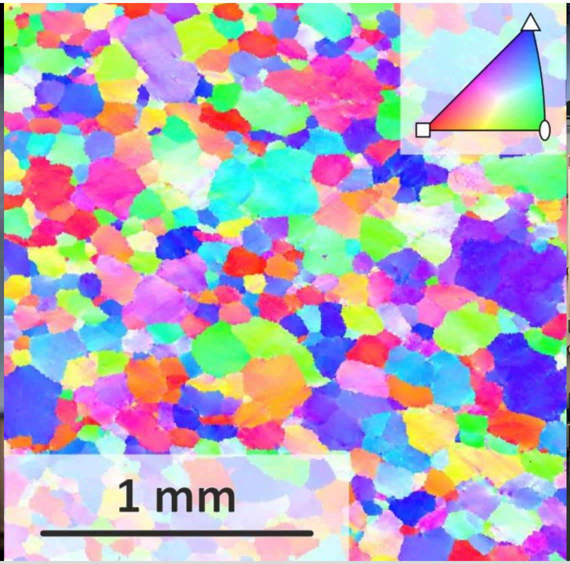
Institute for Applied Materials (IAM-WK)



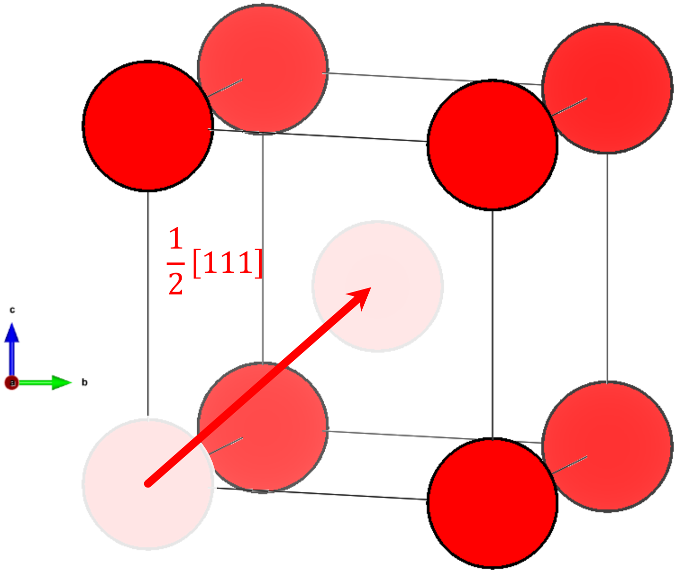


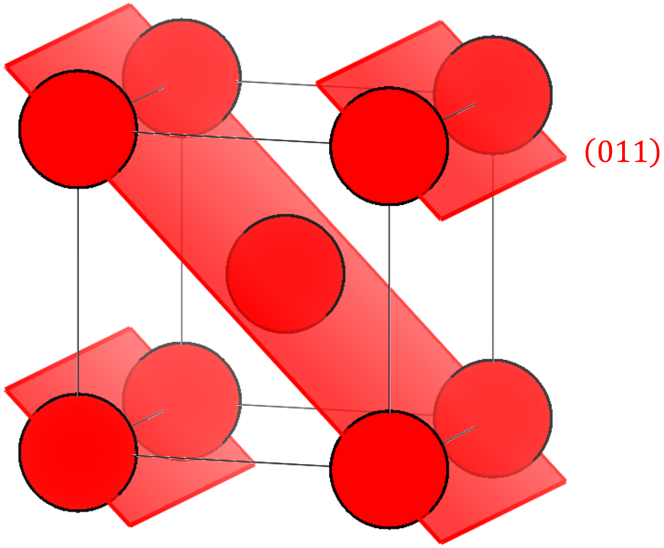
Topics

- Dislocations in Metals and Alloys: A2
  - Pencil Glide
  - Core Configuration of Screw Dislocations
  - Kink Pair Formation and Propagation

Strukturbericht Designation A2

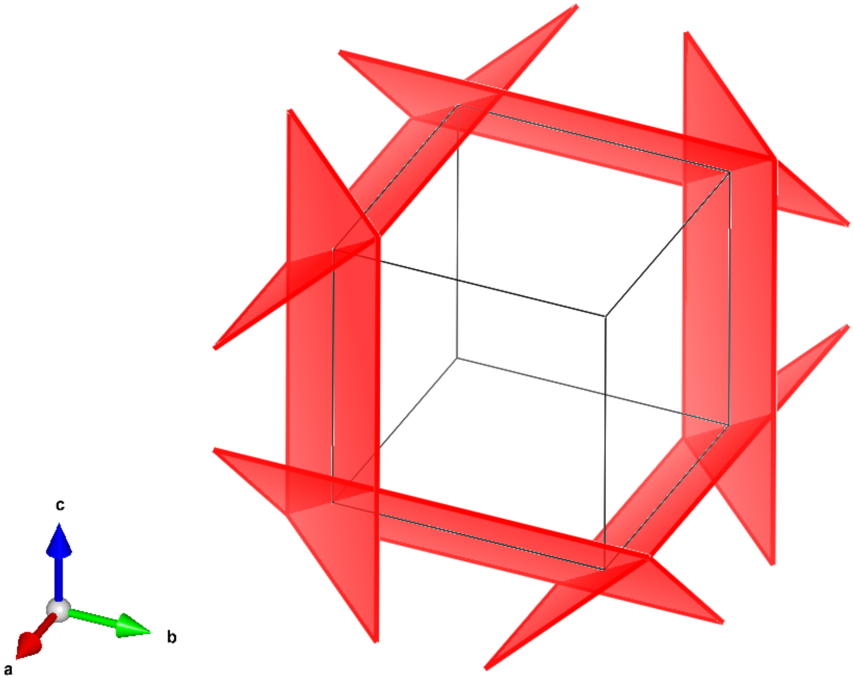
- **Body centered cubic metals and alloys are only densely packed, not closed packed.** Planes with highest packing factor are $\{110\}$. The shortest full lattice translations are along $\frac{1}{2}\langle 111\rangle$. (Remember: use of the conventional cell here.)

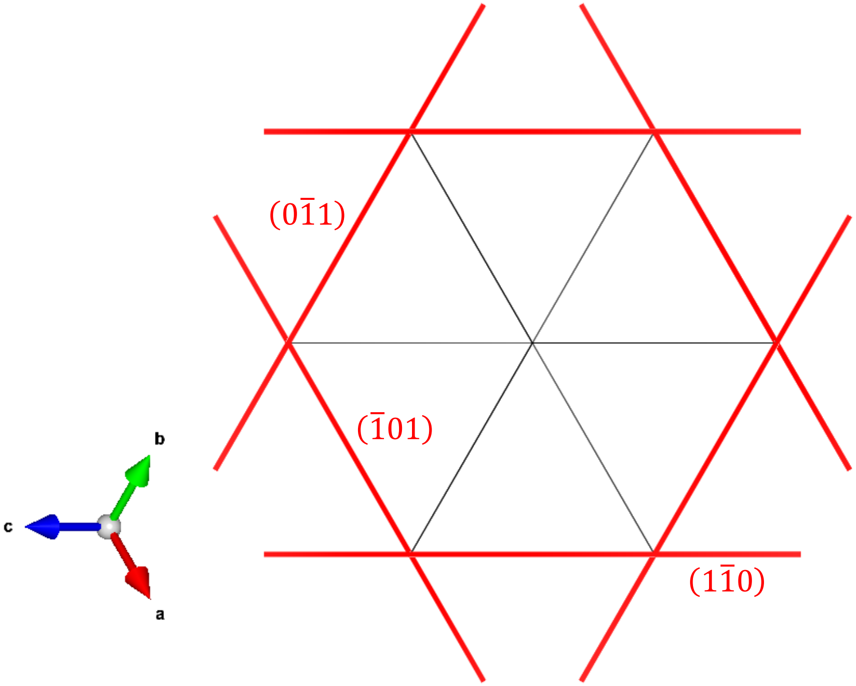




“Pencil Glide”

- $\{110\}\frac{1}{2}\langle 1\bar{1}1\rangle$ are called **pencil glide** systems.

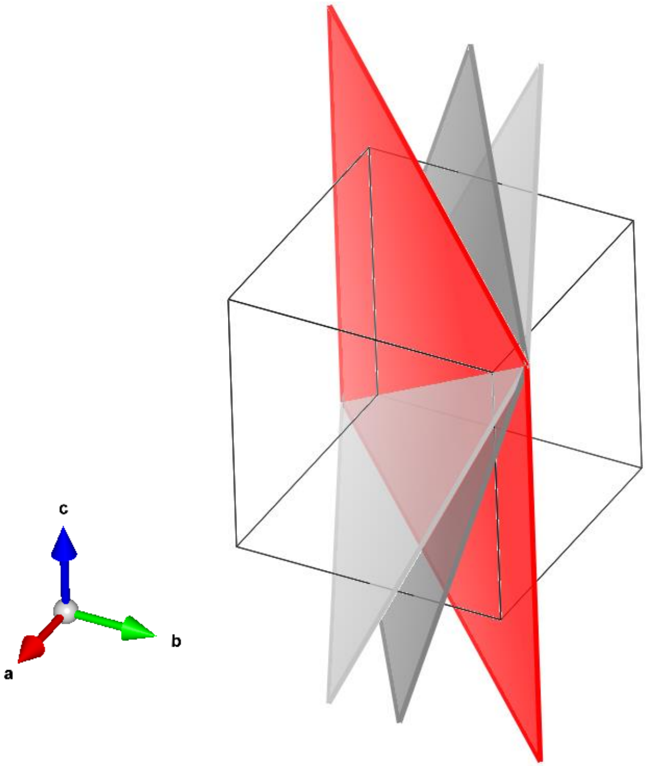


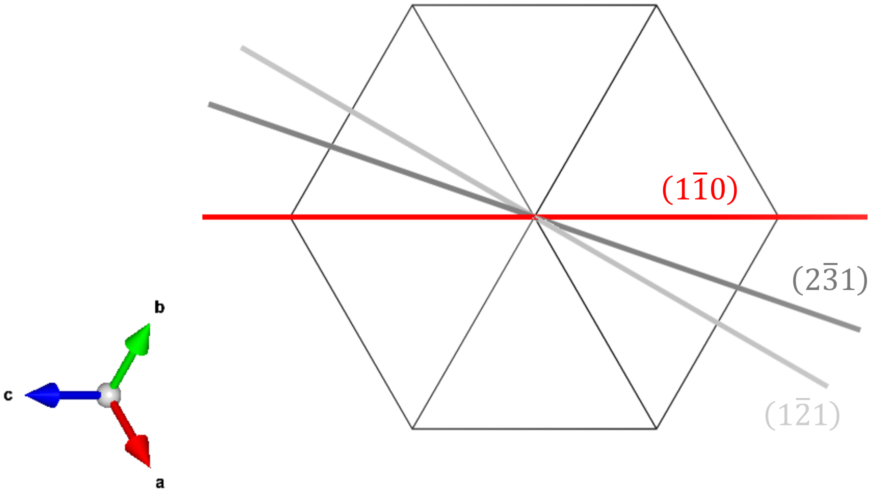


viewing direction: [111]

“Pencil Glide”

- In addition to these systems, other systems with $\frac{1}{2}\langle 1\bar{1}1\rangle$ slip direction are also reported in literature: $\{121\}\frac{1}{2}\langle 1\bar{1}1\rangle$ and $\{132\}\frac{1}{2}\langle 1\bar{1}1\rangle$.





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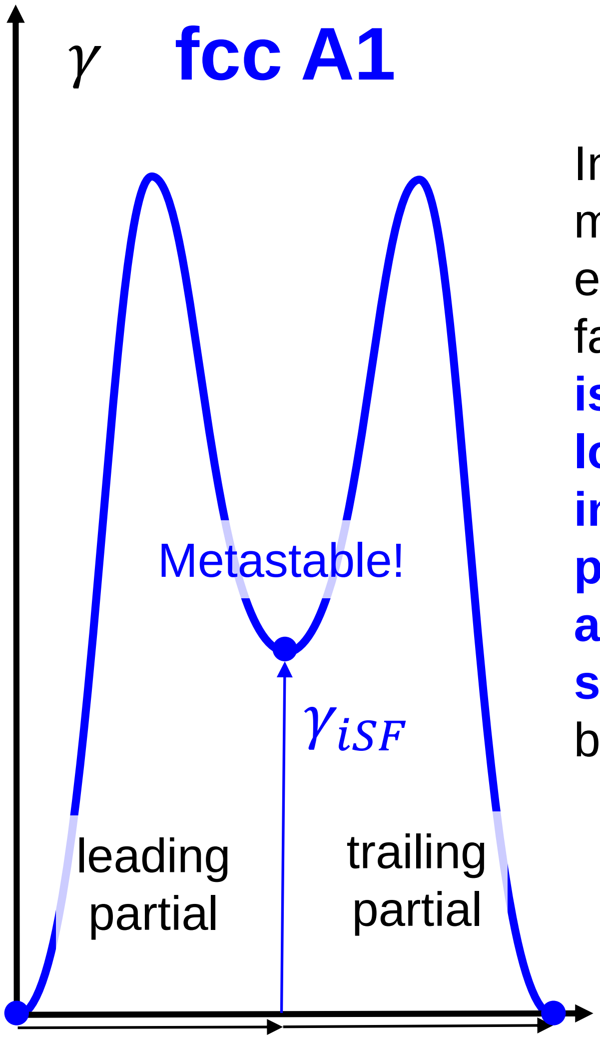
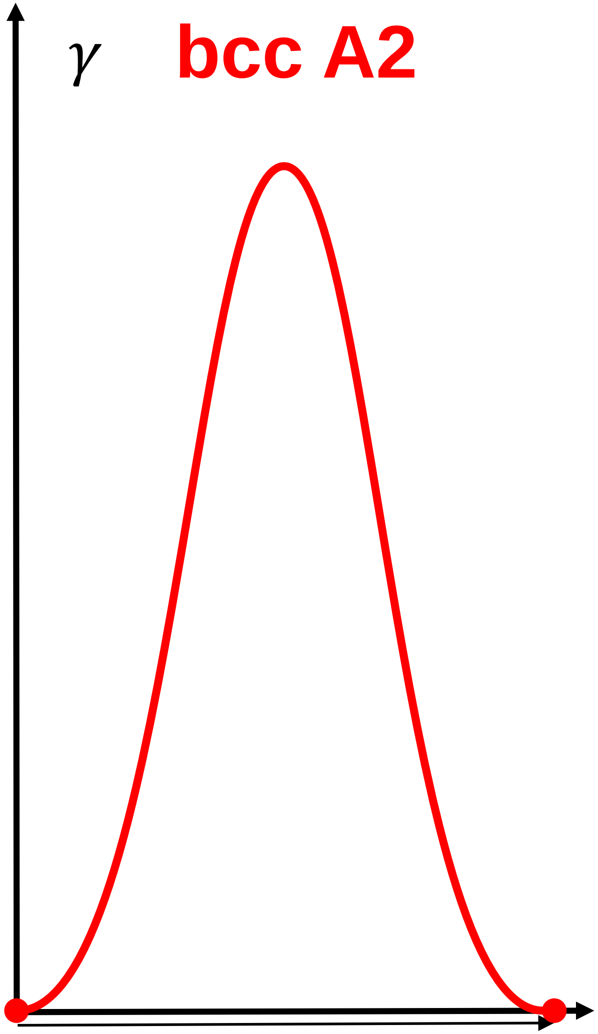
“Pencil Glide”

- For every $\langle 1\bar{1}1\rangle$ slip direction, there are three $\{110\}$ planes, three $\{121\}$ planes and six $\{132\}$ planes.
- In A2 metals and alloys, **a significant probability for cross-slip is observed** which makes the analysis of slip planes by slip traces complicated (macroscopic slip traces might originate from iterative cross-slip processes).
- There are reports on $\langle 100\rangle$ Burgers vectors in dislocation patterns. These might originate from dislocation reactions. Under certain conditions, temperature-depending, anisotropic elasticity can result in a lower line energy of these dislocations in comparison to $\frac{1}{2}\langle 1\bar{1}1\rangle$ dislocations. Under these circumstances, the $\langle 100\rangle$ Burgers vectors might also be observed during plastic deformation without special reactions needed.
- **There are no metastable stacking faults in bcc metals!** Hence, there is nothing such as the dissociation of dislocations as in fcc A1 metals and alloys. This is consistent with the strong tendency for cross-slip in bcc A1 metals and alloys.

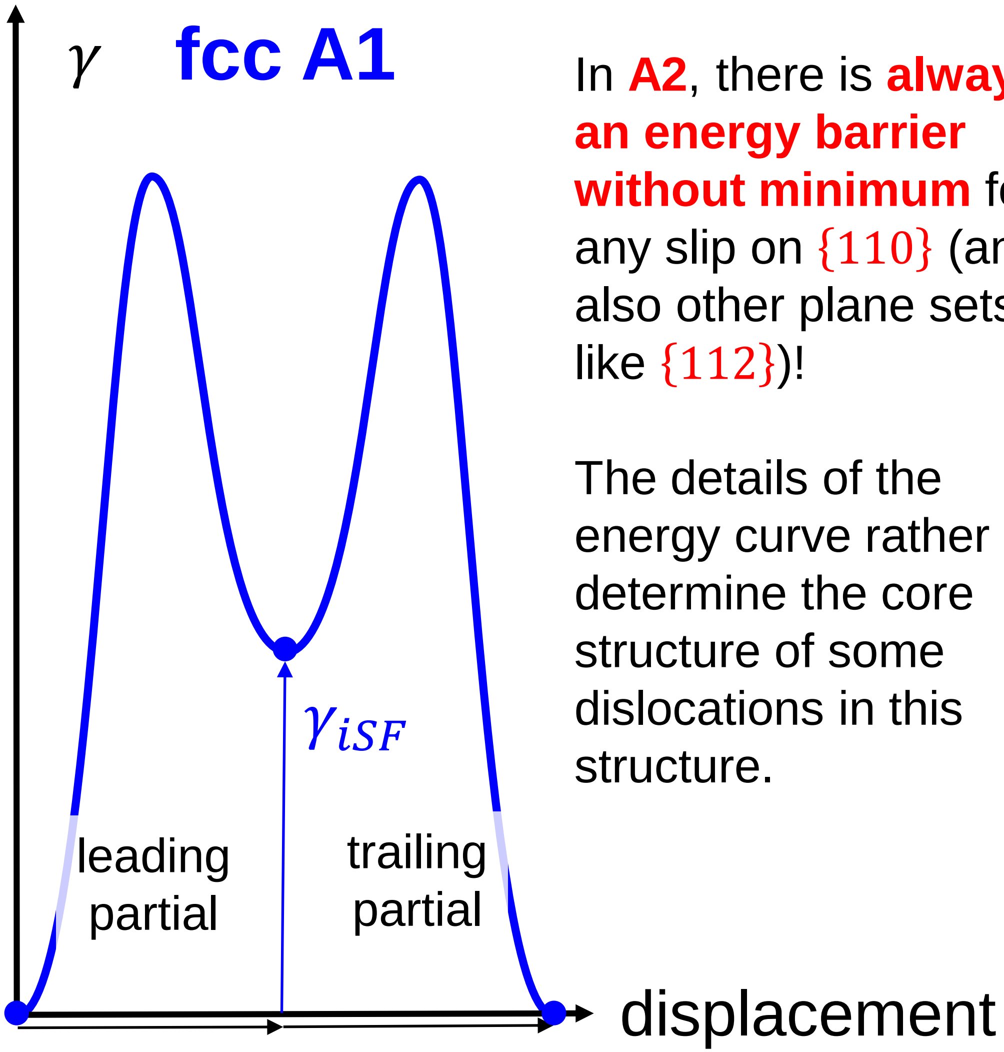
Stacking Faults



In **A1**, there is a metastable minimum energy of the stacking fault. The **dissociation is determined by the long-range elastic interaction of the partial dislocations and the intrinsic stacking fault** in between.

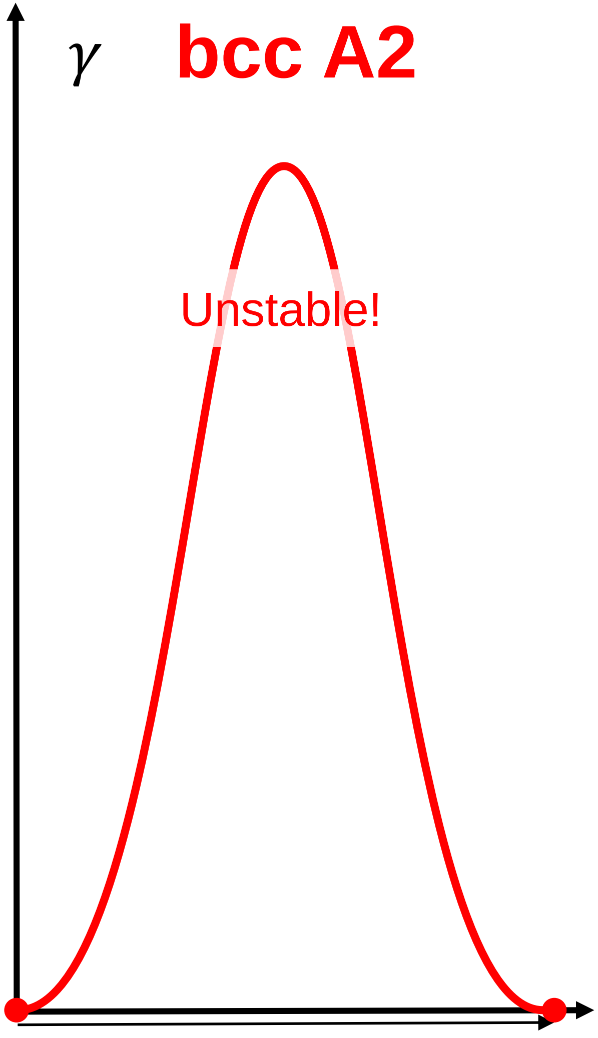


Stacking Faults



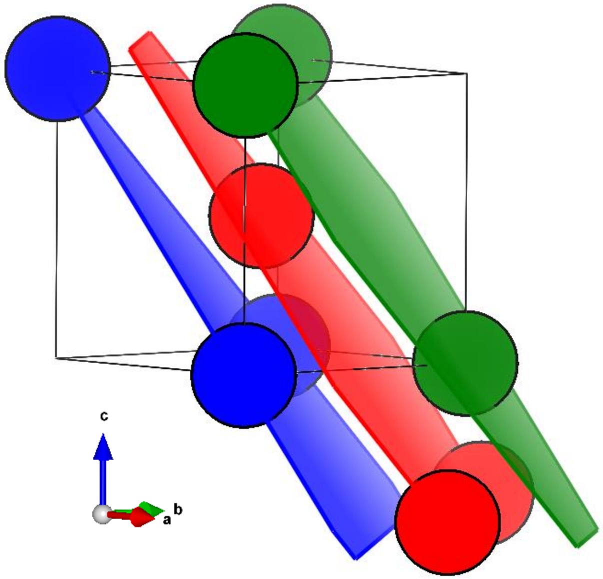
In **A2**, there is **always an energy barrier without minimum** for any slip on $\{110\}$ (and also other plane sets like $\{112\}$)!

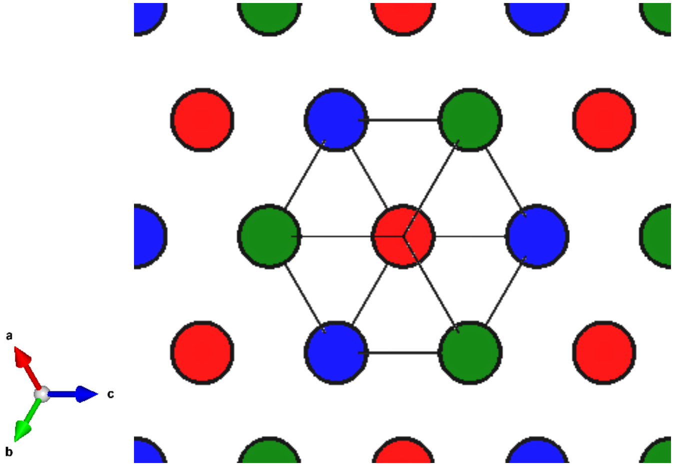
The details of the energy curve rather determine the core structure of some dislocations in this structure.



Core Structure of Screw Dislocations

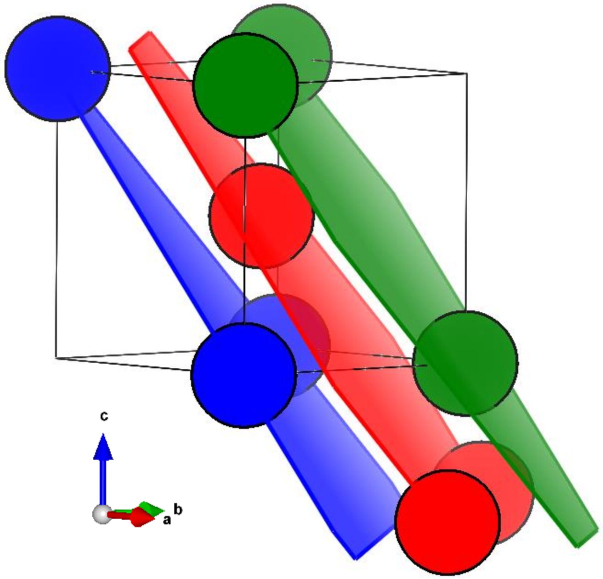
- In order to visualize the core structures of screw dislocations, a special projection along the dislocation line is used. Hence, the dislocation line and the Burgers vector $\boldsymbol{b} = \frac{1}{2}\langle 111 \rangle$ **are out-of-plane**.
- $\{111\}$ **planes are spaced by** $b/3$. There are **three different atomic positions** from these planes.

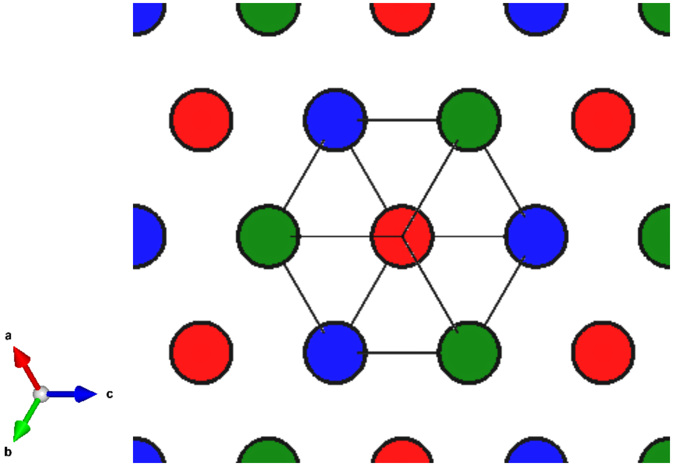




Core Structure of Screw Dislocations

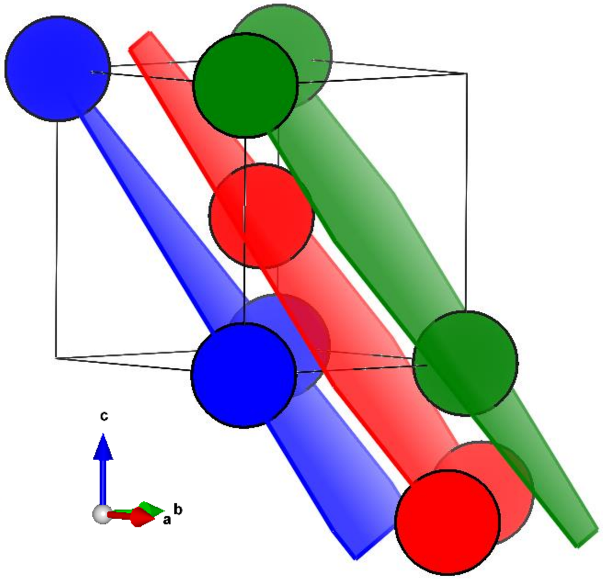
- **The displacement field of the screw dislocation is not visible directly from atom positions in this plot** since all displacements are out-of-plane, only. It’s essentially the same for the perfect and distorted crystal.
- The disregistry is visualized by incorporating the changes of the connections of nearest neighbor atoms. **The arrows indicate direction and magnitude (by the scale) of change of the nearest neighbor connections by displacement along $\langle 111\rangle$.** When change in length falls between $b/2$ and b, the size is reduced by b.

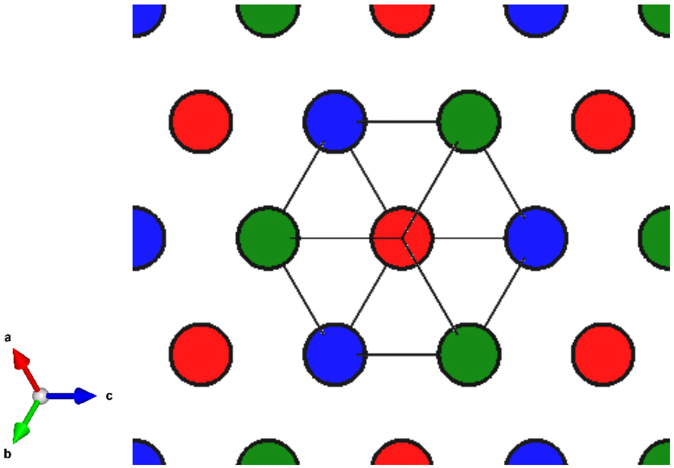




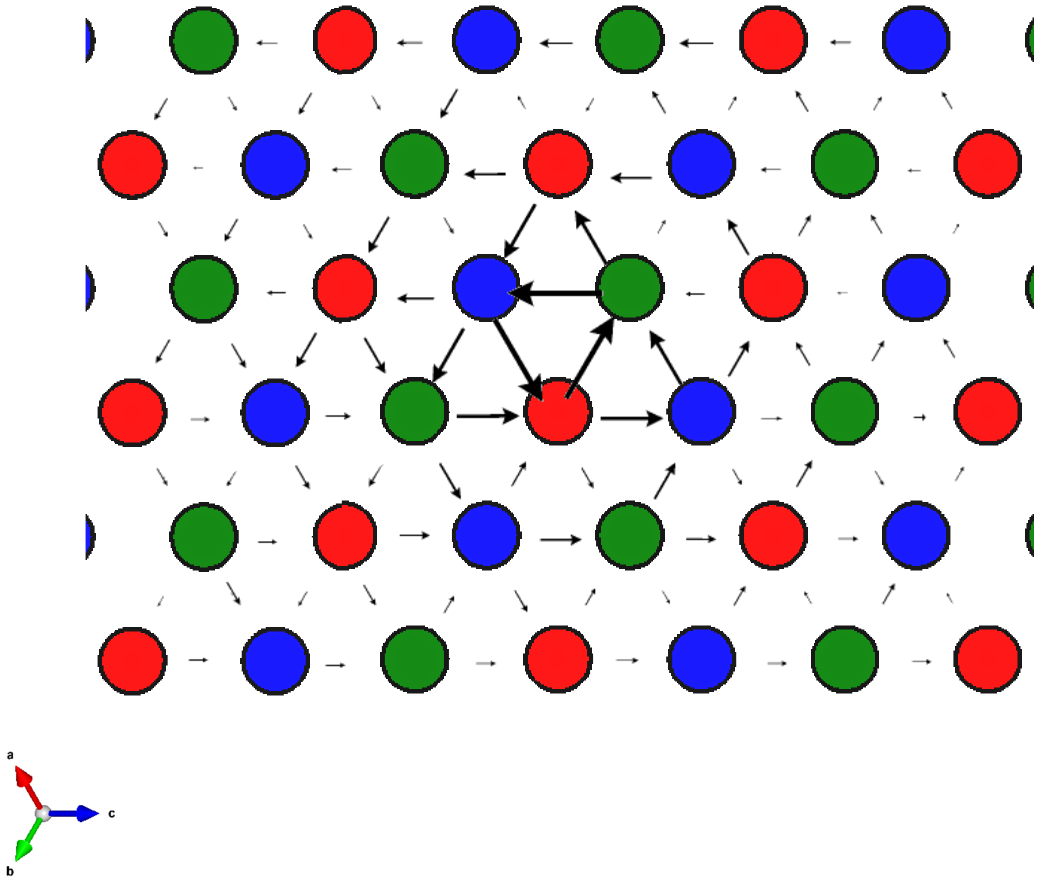
Core Structure of Screw Dislocations

- The simple Ansatz from Ch. 4c with $u_z = \frac{b}{2\pi}\tan^{-1}(y,x)$ leads to arrows‘ length declining rapidly with increasing r ($\sim {}^{1}/_{r}$). The symmetry is circular.



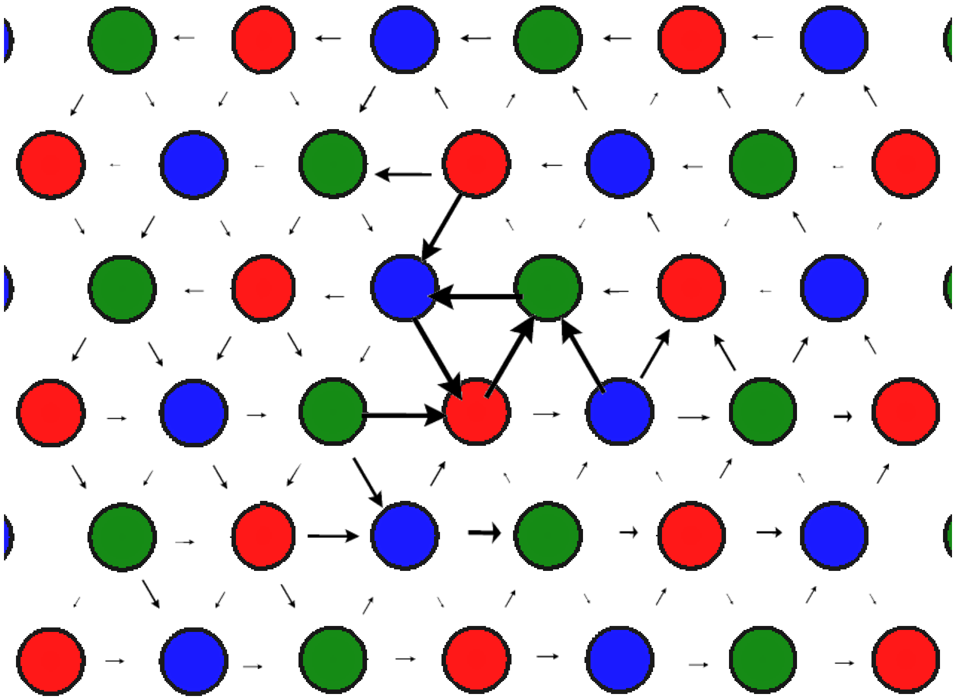


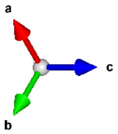
Core Structure of Screw Dislocations



- Instead of a circular symmetry, computational methods revealed **concentrations of the displacements in adjacent $\{110\}$ planes of the zone axis.**
- The **distribution of the displacements correlates with the principle symmetry of the crystal** here: all configurations follow the $\bar{3}$ **along the $\langle 111 \rangle$ zone axis**.
- In the **"non-degenerated"** configuration, the second symmetry operation with 2 **along the $\langle 110 \rangle$ in the projection plane** is also fulfilled.

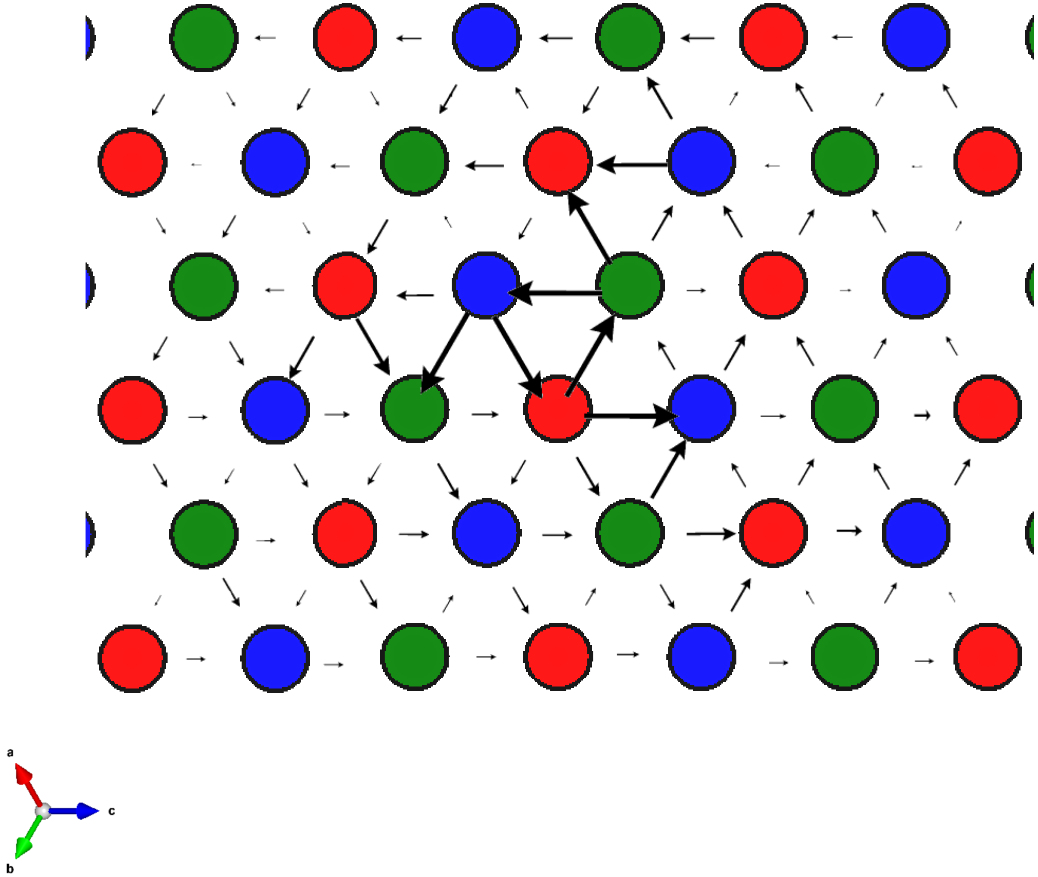
Core Structure of Screw Dislocations





- The **“degenerated”** configuration breaks the symmetry by the 2 **along the** $\langle 110 \rangle$ **in the projection plane.**

Core Structure of Screw Dislocations

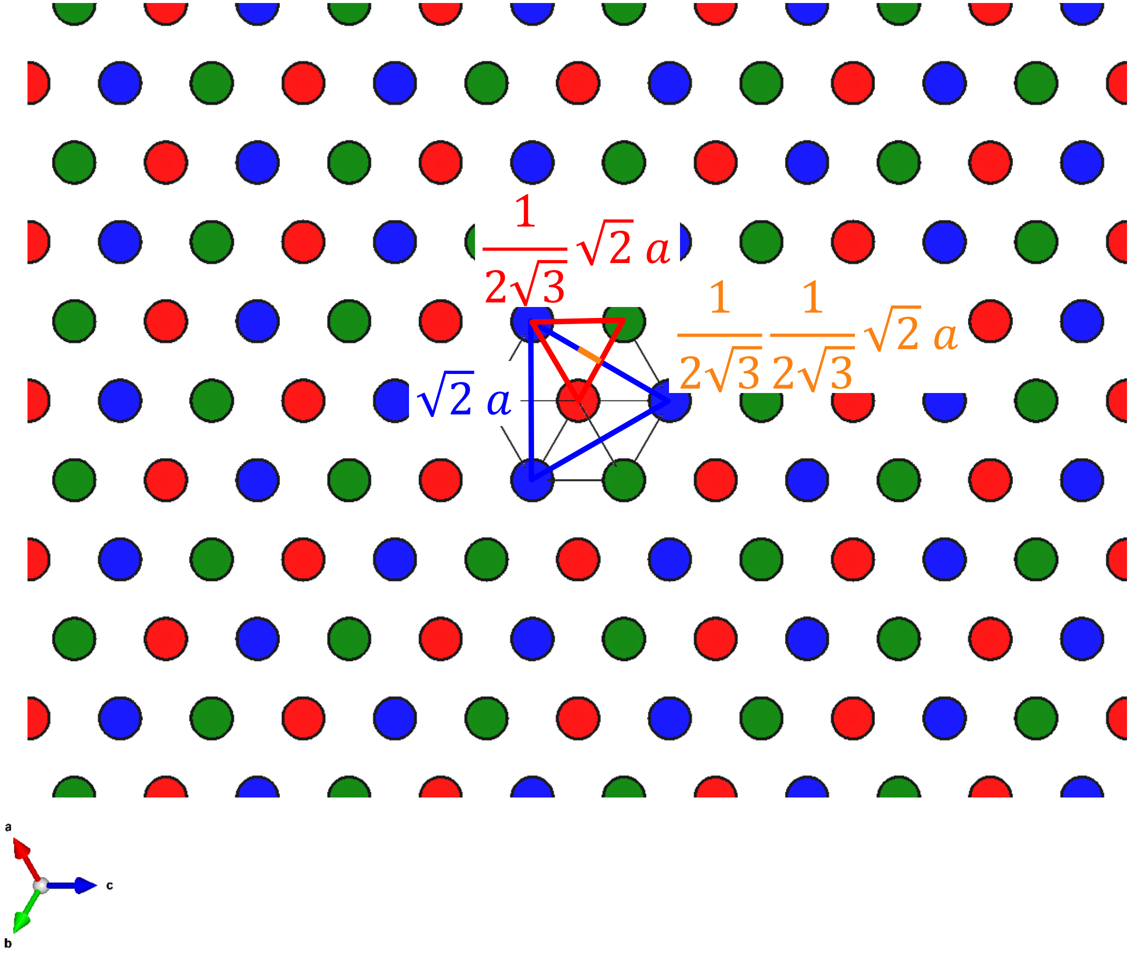


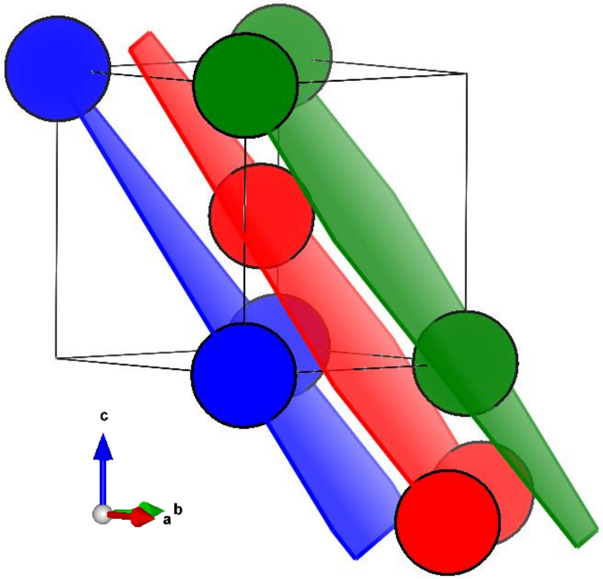
- There are two enantiomorphic possibilities of the “degenerated” configuration.

Core Structure of Screw Dislocations

- **There is a concentration of displacements in three adjacent $\{110\}$ planes, but there is no dissociation in the sense of a metastable stacking fault and elastically interacting partial dislocations.**
- **The distinct atomic arrangement in the core is sensible against tiny difference in the interatomic potentials.**
- **The relaxed core structure of screw dislocations leads to a significant reduction in core energy contribution of the screw dislocation**:
  - In conjunction with the anyway smaller elastic energy of screw dislocations, a significant preference of screw character is observed in bcc metals and alloys.
  - Furthermore, specific positions of he screw dislocation core are preferred. The energy barriers for dislocation motions are high.
- Enantiomorphic core configurations might cause a direction depending critical on-set stress for dislocation motion.

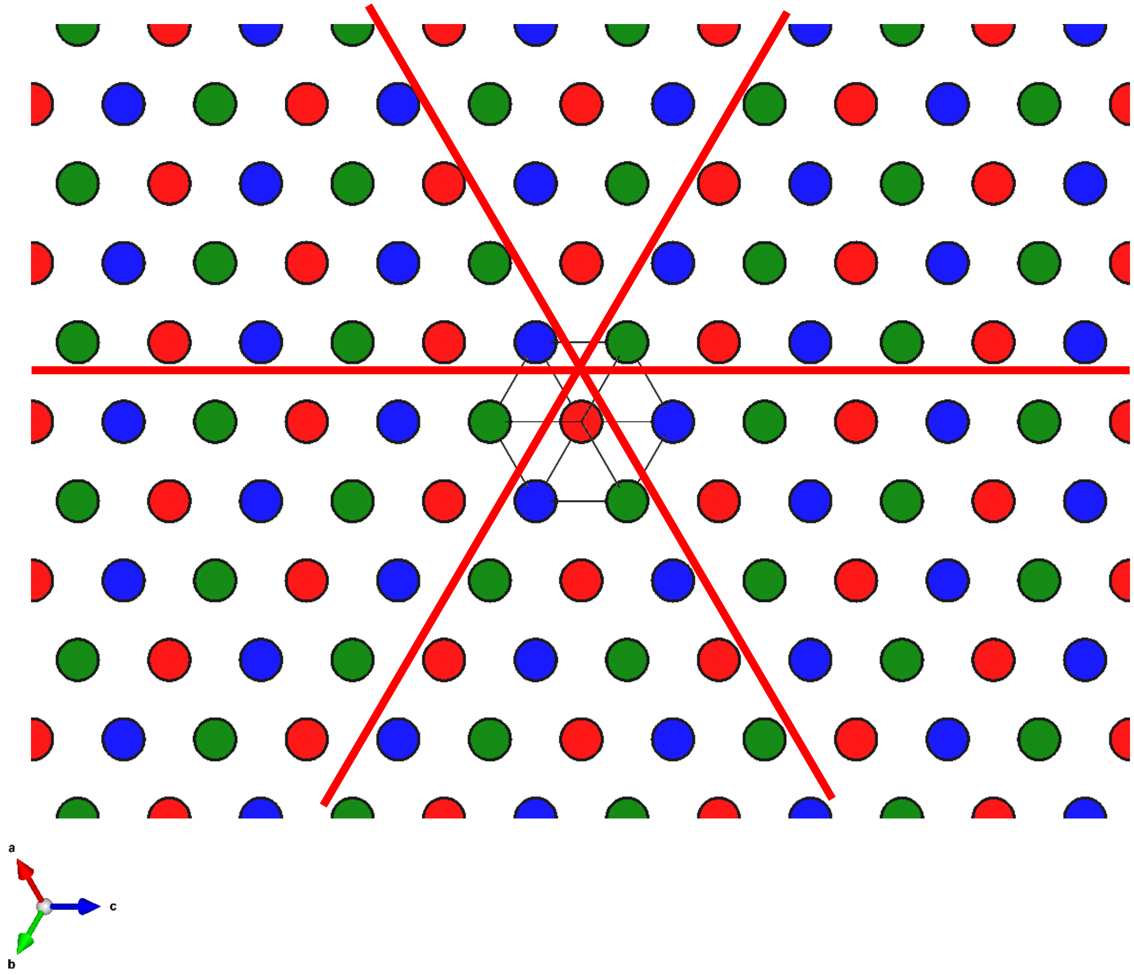
Core Structure of Screw Dislocations

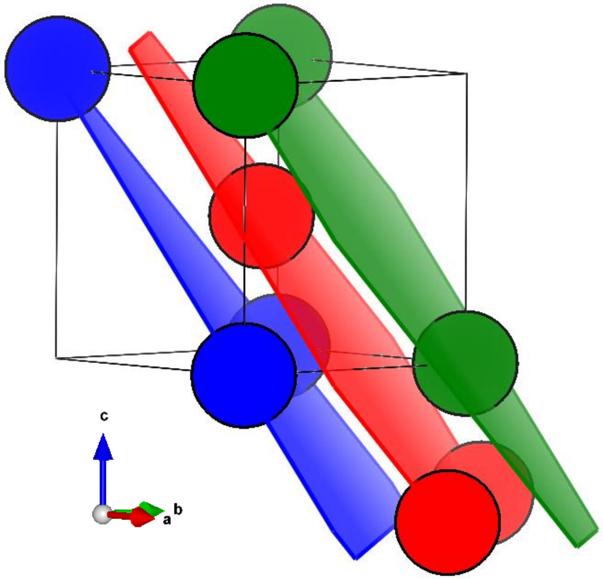


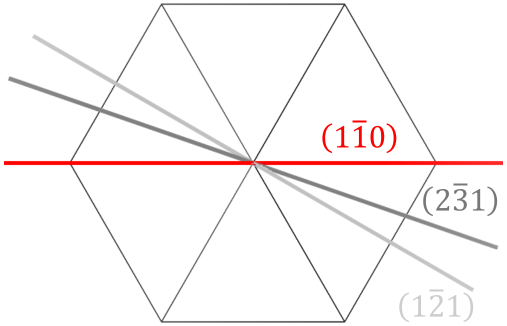


Core Structure of Screw Dislocations

Not connecting two center positions of the relaxed core structures!

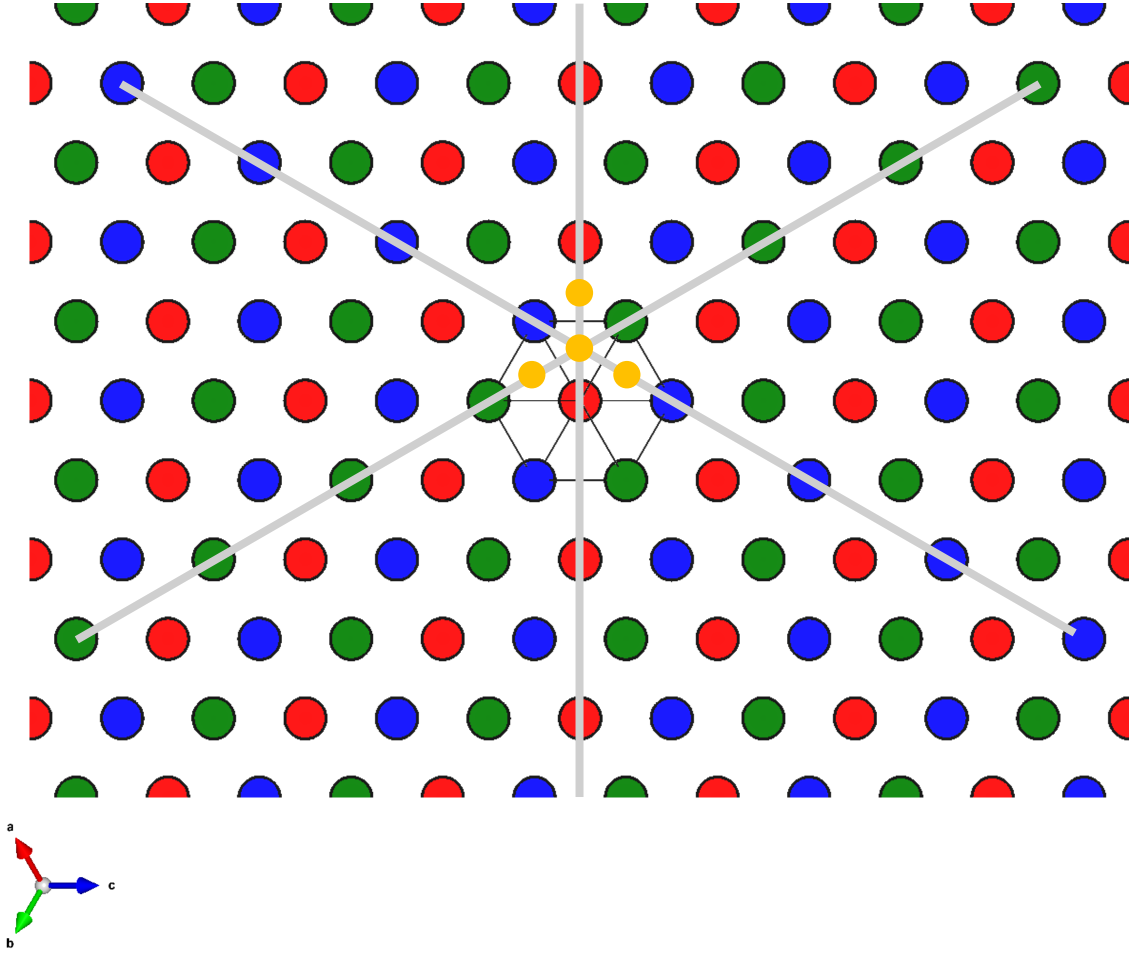


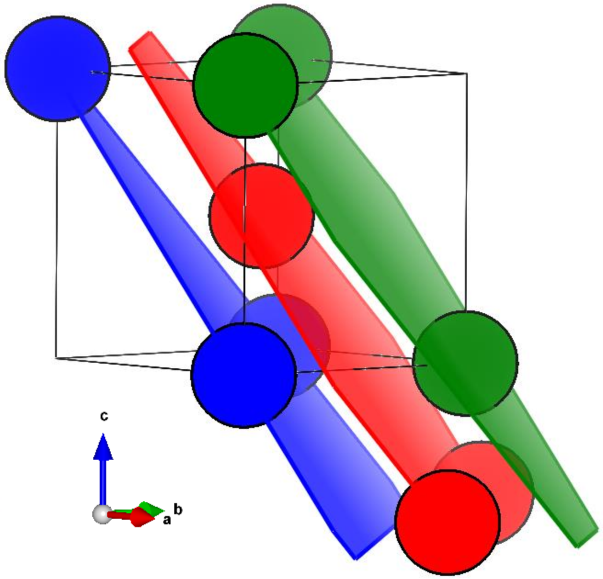


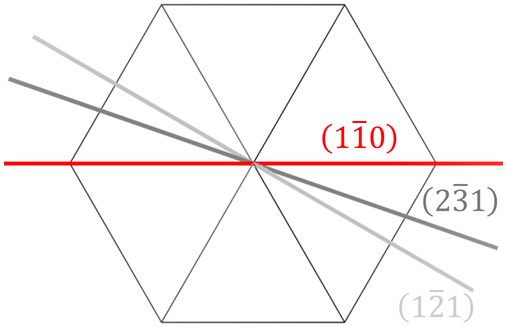


Core Structure of Screw Dislocations

Connecting two center positions of the relaxed core structures!



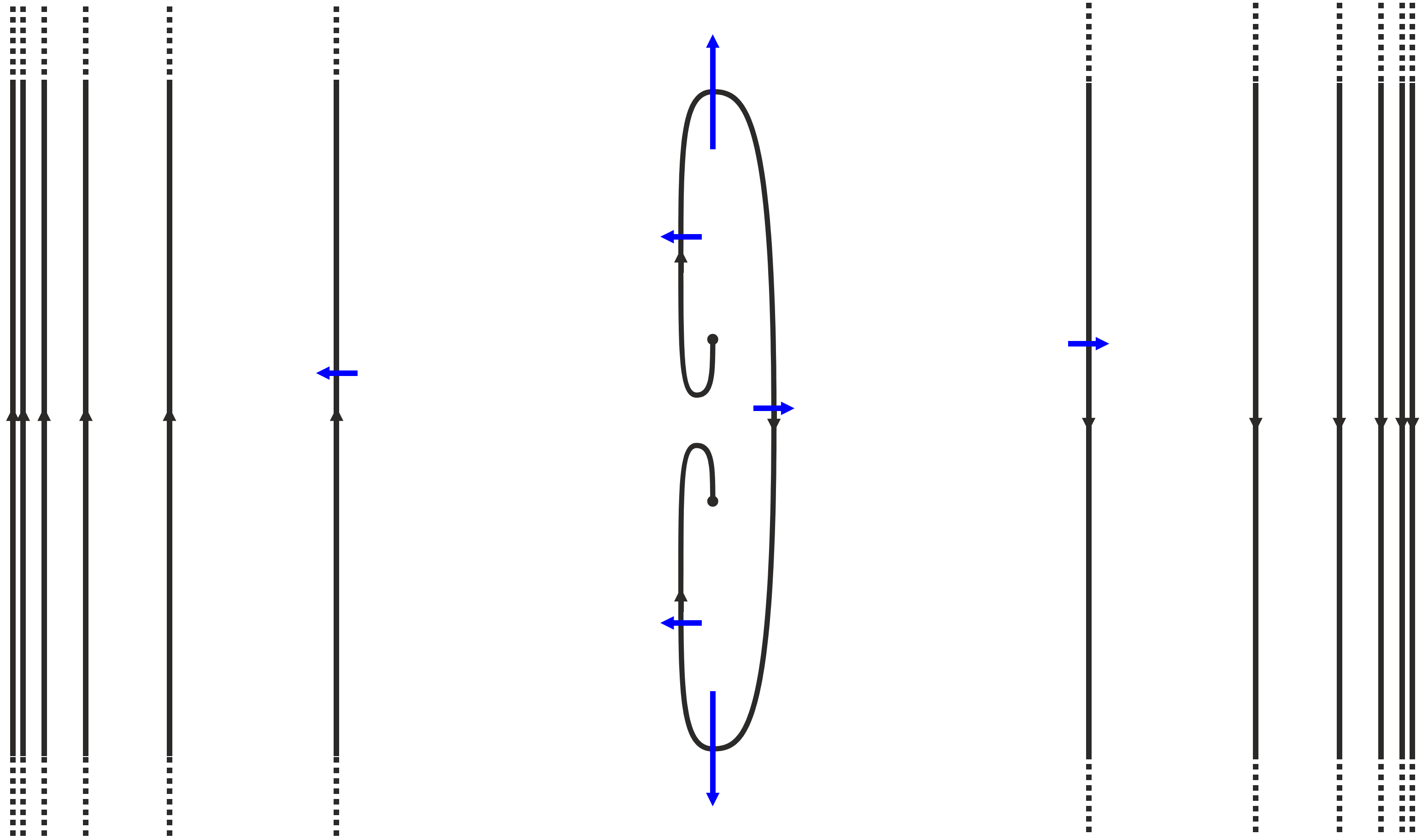




Consequences

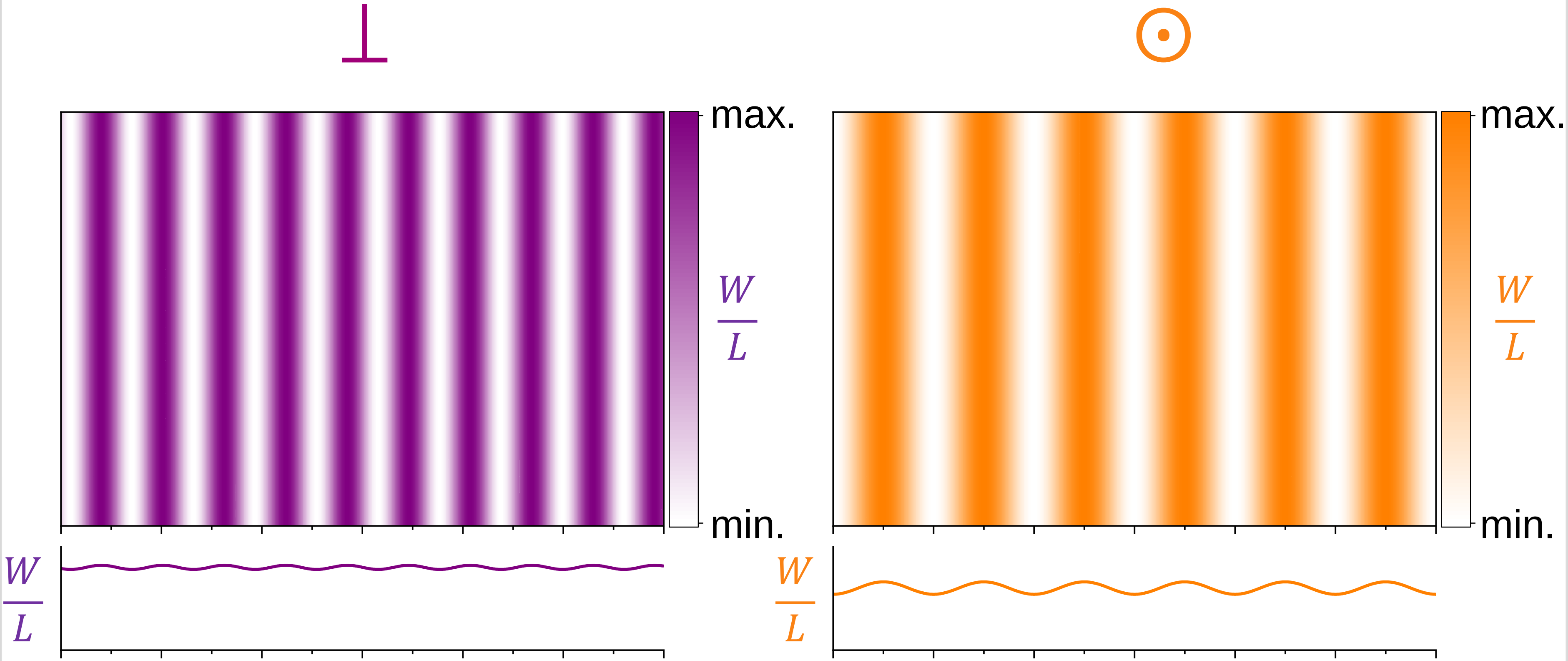
- Most dislocations are of screw character in A2 metals and alloys.
- There are high on-set stresses for screw dislocation motion. Other dislocation segments quickly run out!
- **Macroscopic yielding of A2 metals and alloys is often determined by the on-set of significant screw dislocation motion. (If edge dislocation mobility is not slowed down by other factors.)**

Consequences



Glide source in an A2 metals. Long screw segments are formed by fast moving edge components. Low-mobility screw dislocations pile-up and may block the source. Further plastic deformation depends on screw dislocation motion.

Kink Pairs

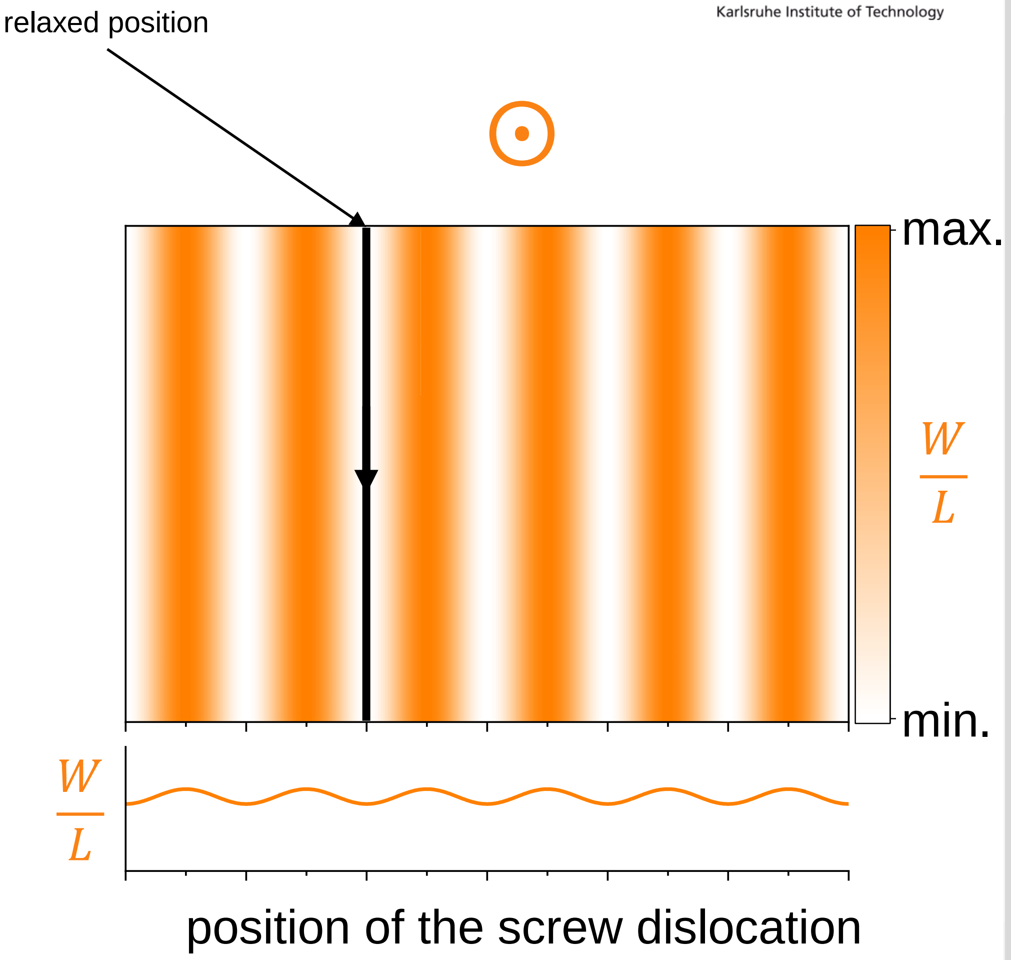


position of the edge dislocation

position of the screw dislocation

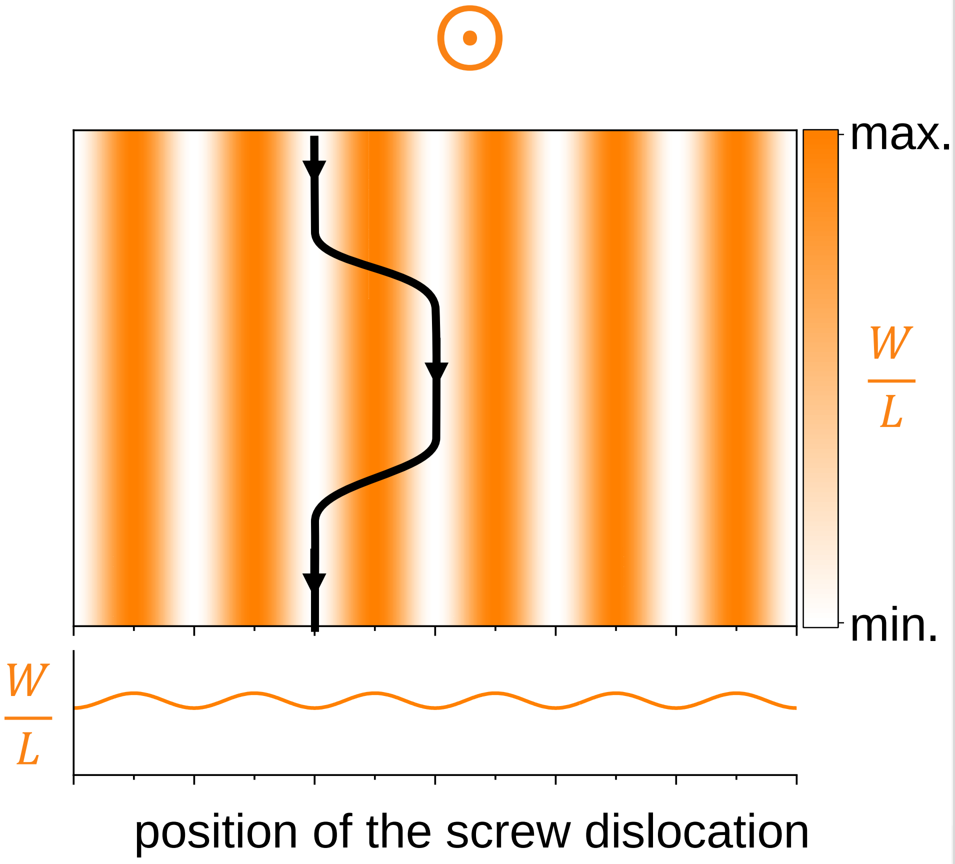
Kink Pairs

- The **movement of the screw dislocations** is mediated by **thermally activated kink pair formation and propagation**.
- At finite temperature, **thermal fluctuations** lead to the **spontaneous formation of kink pairs**. The probability for the formation scales with an Arrhenius factor.
- **Under external load, the kink pairs can propagate** and lead to a motion of the dislocation line to the adjacent potential minimum.



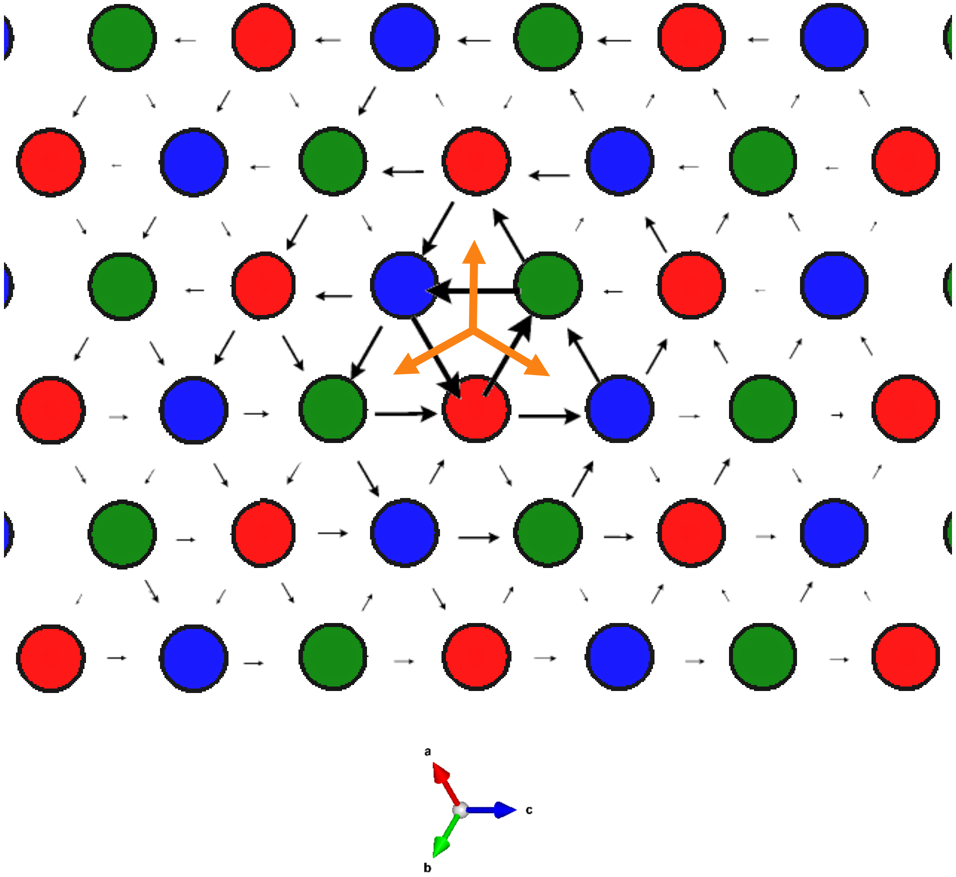
Kink Pairs

- The mathematical treatment contains following important contributions:
  - **Energy barrier between the minima**
  - **Line tension forcing the dislocation line to be straight**
  - **Interaction energy of the antiparallel kinks**
- **Since the process is thermally activated, the a significant temperature and strain rate dependence is observed.**



Kink Pairs

- All adjacent energy minima are equal for no external load! Hence, there is a strong tendency for cross-slip.



Summary

- In A2 metals and alloys, **slip systems with $\langle 111 \rangle$ slip direction are active.**
- **The core structure of screw dislocations can relax by distribution of the disregistry into adjacent $\{110\}$ planes.**
- **This causes strong Peierls barriers against the motion of screw dislocations. The yield strength of A2 metals and alloys is therefore governed by the on-set of significant screw dislocation motion. The motion of screw dislocations itself is thermally activated and mediated by kink pair formation and propagation.**