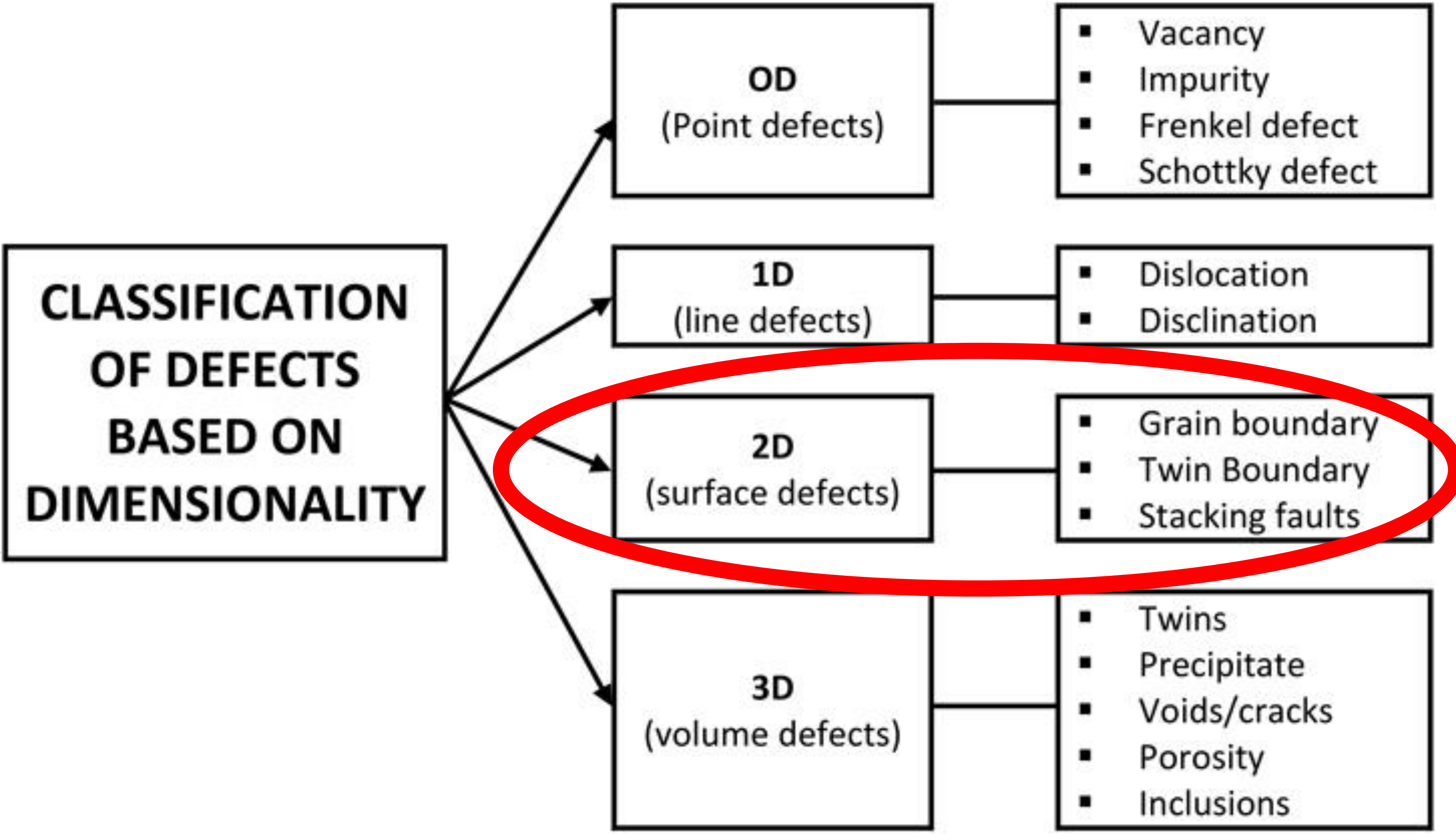


CLASSIFICATION OF DEFECTS BASED ON DIMENSIONALITY

OD
(Point defects)

- Vacancy
- Impurity
- Frenkel defect
- Schottky defect

1D
(line defects)

- Dislocation
- Disclination

2D
(surface defects)

- Grain boundary
- Twin Boundary
- Stacking faults

3D
(volume defects)

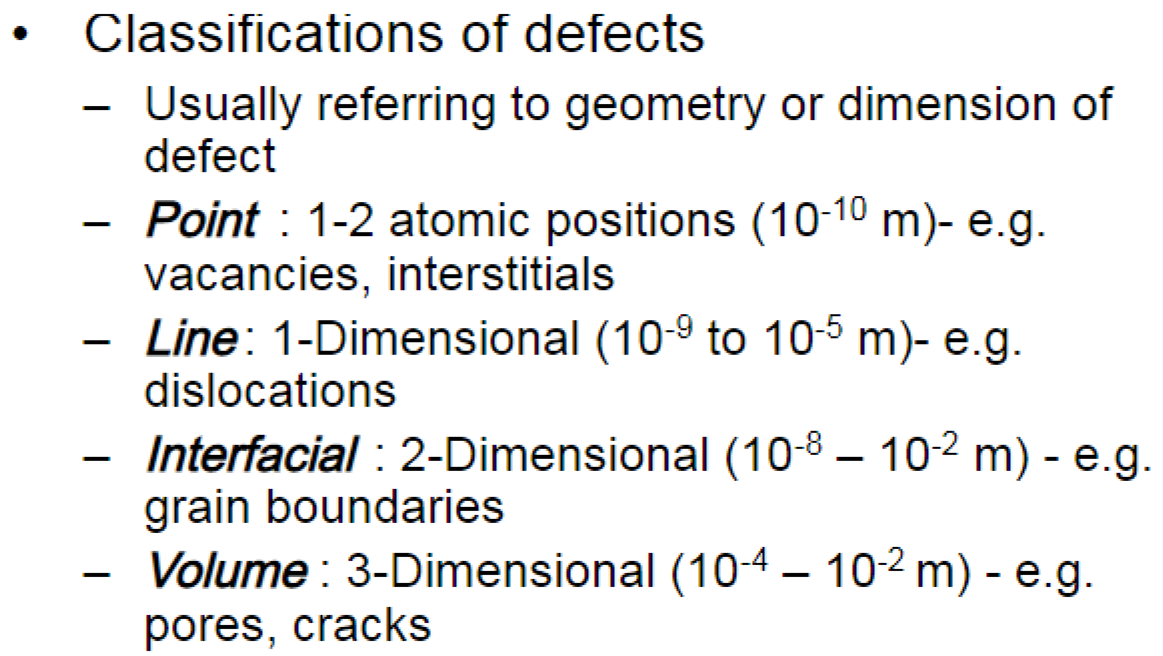
- Twins
- Precipitate
- Voids/cracks
- Porosity
- Inclusions

(2D) SURFACE (INTERFACIAL) DEFECTS

Interfacial defects are boundaries that have two dimensions and normally separate regions of the materials that have different crystal structures and/or crystallographic orientations.

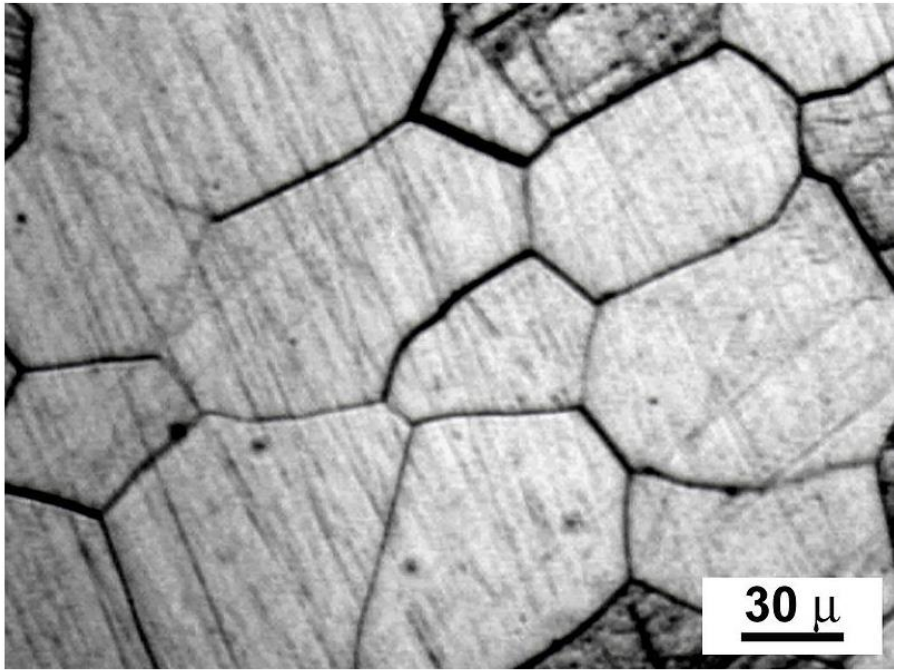
These imperfections includ

- external surfaces
- grain boundaries
- phase boundaries
- twin boundaries
- stacking faults.



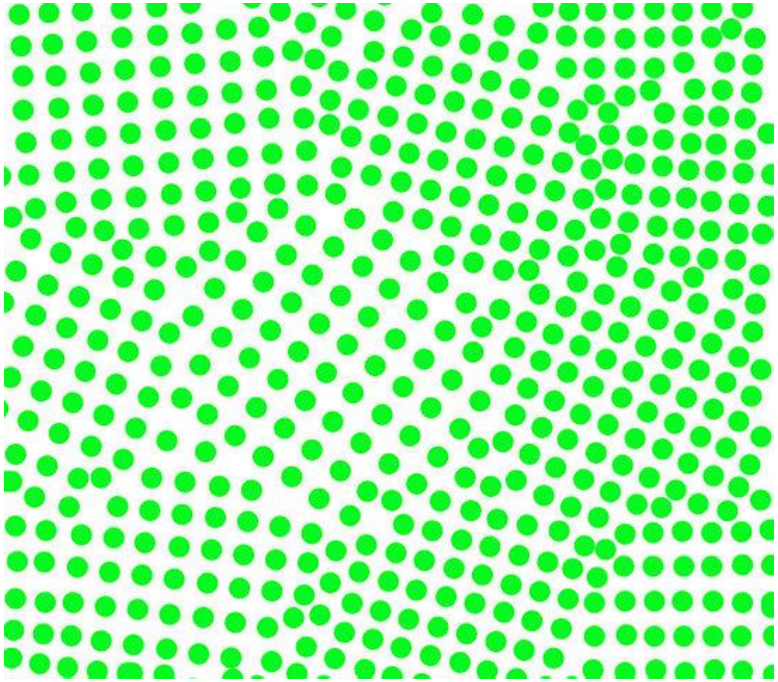
- Classifications of defects
  - Usually referring to geometry or dimension of defect
  - ***Point*** : 1-2 atomic positions (10^{-10} m)- e.g. vacancies, interstitials
  - ***Line***: 1-Dimensional (10^{-9} to 10^{-5} m)- e.g. dislocations
  - ***Interfacial*** : 2-Dimensional (10^{-8} – 10^{-2} m) - e.g. grain boundaries
  - ***Volume*** : 3-Dimensional (10^{-4} – 10^{-2} m) - e.g. pores, cracks

2D, Planar defects: the interfaces between homogeneous regions of the material (e.g. grain boundaries, stacking faults, external surfaces)



Micrograph of a polycrystalline metal; grain boundaries evidenced by acid etching.

Microstructure of VT22 (Ti5Al5Mo5V1,5Cr) after quenching



Schematic representation of polycrystalline material consisting of crystallites

Differently oriented crystallites in a polycrystalline material

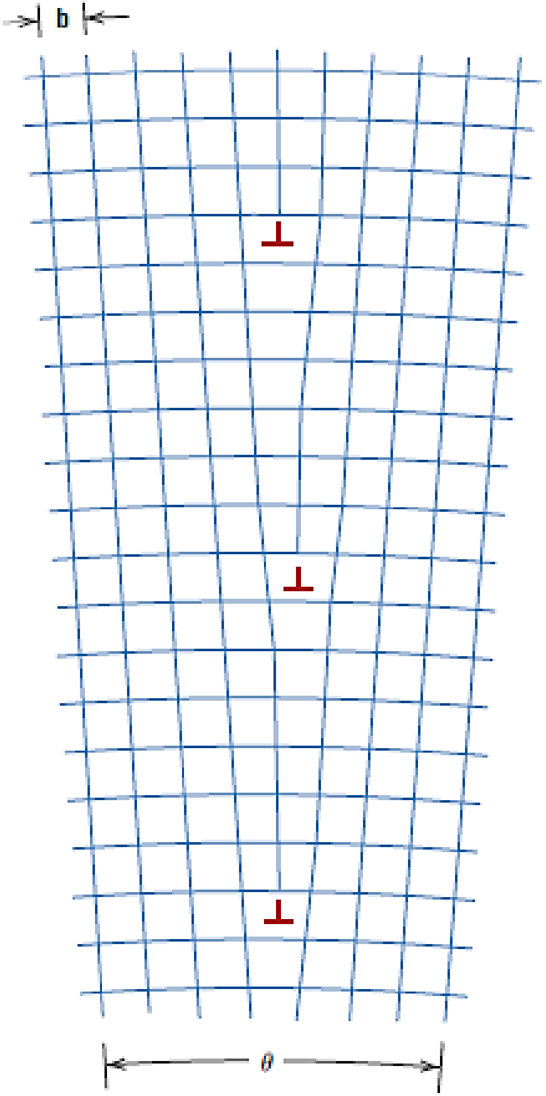
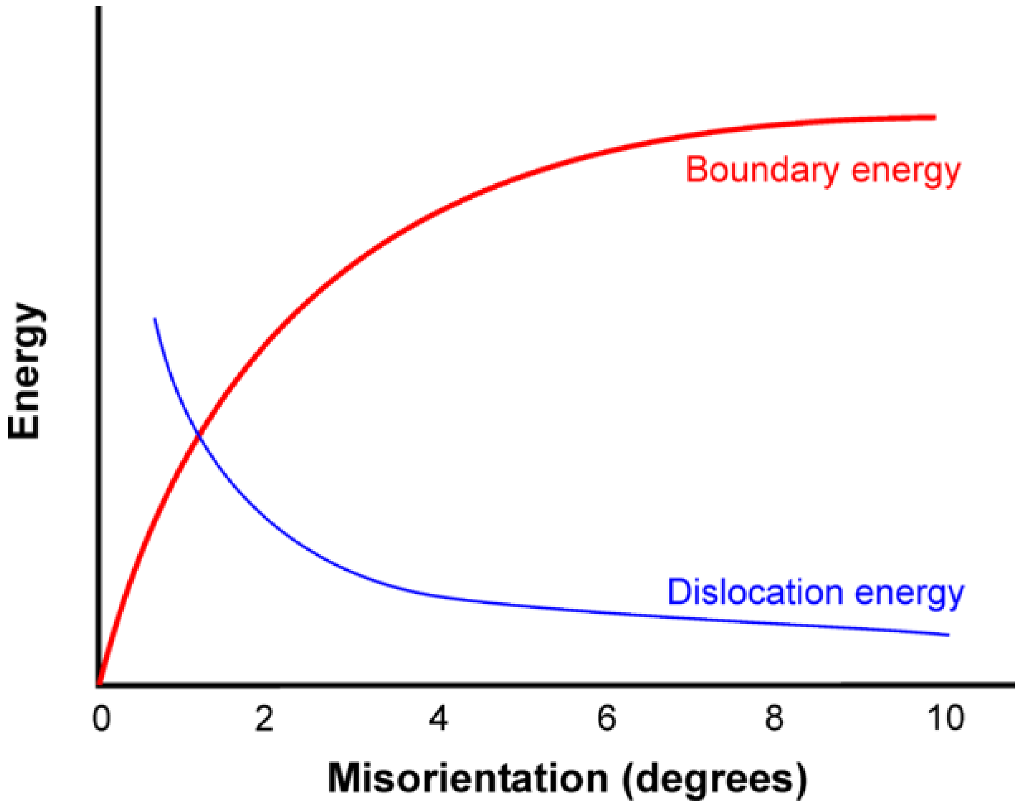


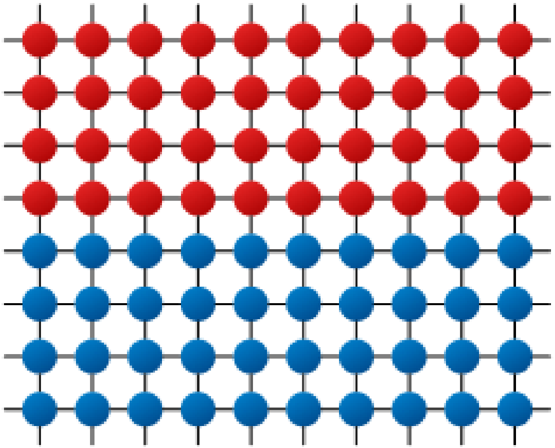
Fig. Demonstration of how a **tilt boundary** having an angle of misorientation u results from an alignment of edge dislocations.

Boundary energy

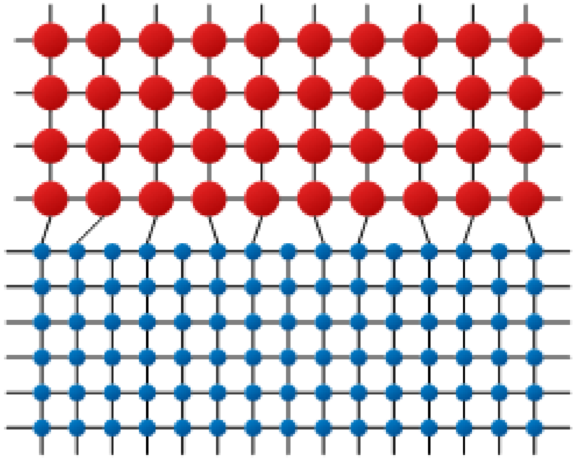


The energy of a tilt boundary and the energy per dislocation as the misorientation of the boundary increases

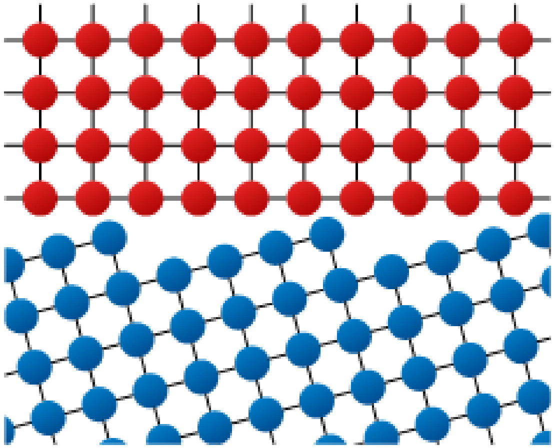
Phase Boundaries



coherent phase boundary



partially coherent phase boundary



incoherent phase boundary

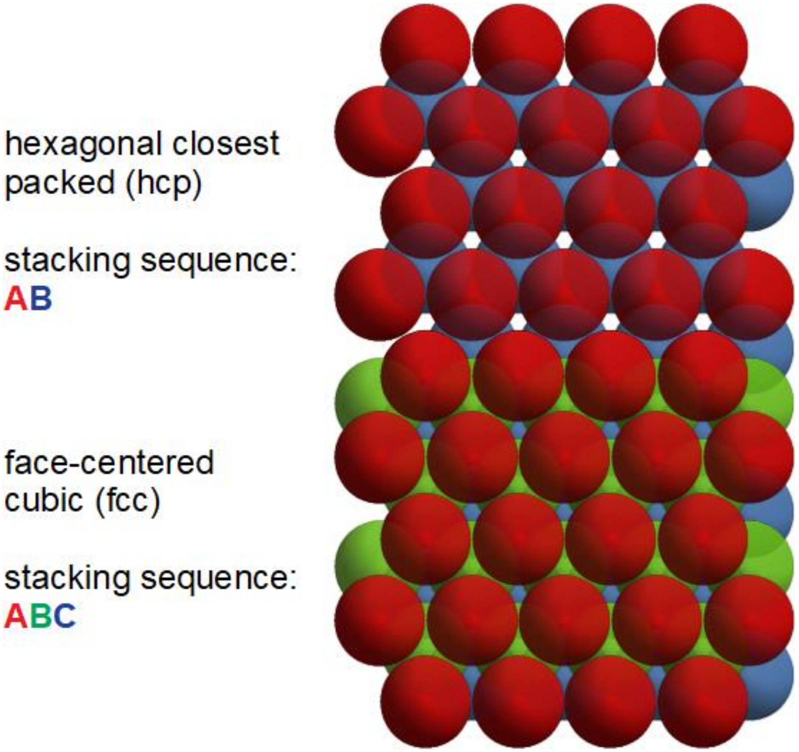
With a **coherent phase boundary**, the two structures merge into one another without any gaps. This is true if the two phases have a consistent structure and similar chemical properties.

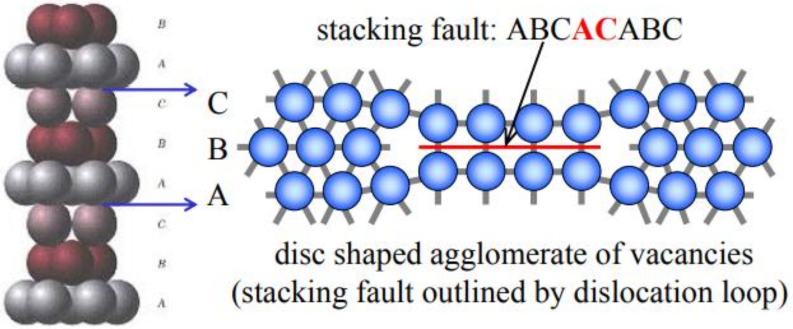
However, if the phases differ somewhat in their properties, the lattice structures no longer completely merge into one another. Therefore dislocations must be present at regular intervals. One then speaks of a **partially coherent phase boundary**..

By contrast, with an **incoherent phase boundary**, neither the lattice structures nor the chemical properties of the two phases match. The structure is similar to a high angle grain boundary, but consists of two distinct phases. The phase boundaries are not distorted to the extent that is the case with high angle grain boundaries.

Stacking fault

Another planar defect is the so-called **stacking fault**. It is a locally different stacking sequence of otherwise periodically arranged planes. For example, the stacking sequence of the closest packed planes in the face-centered cubic lattice with normally ABCABC may locally have the sequence ABACAB. Such stacking faults can arise when a dislocation is split into two smaller dislocations.



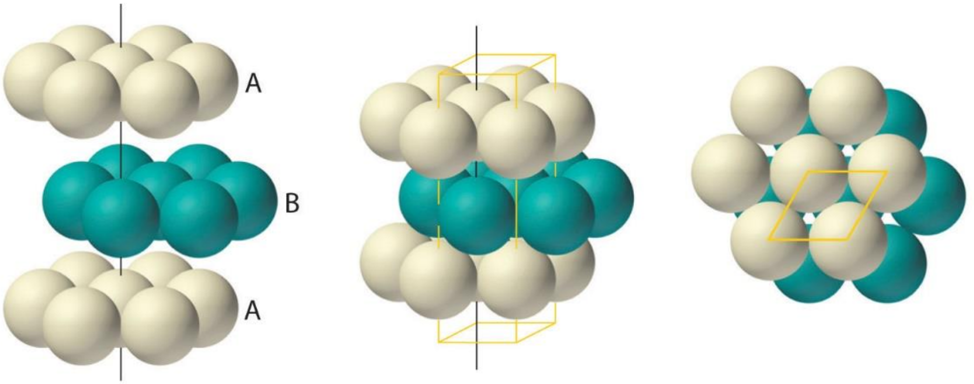


Stacking faults are local deviations from the actual stacking sequence of the lattice structure!

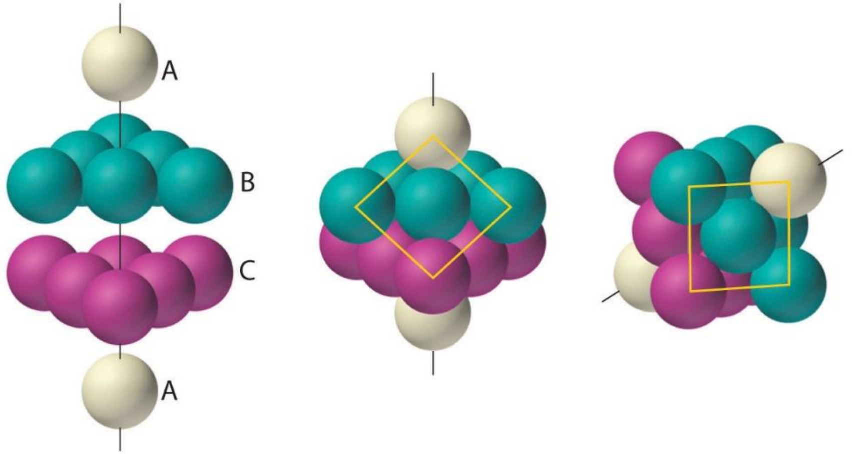
we generated simple crystals (with just one atom per lattice point) by stacking spheres in exactly the way you would do when you put up a mound of oranges or cannon balls. You start by arranging the spheres on a plane as densely as you can. Than you start the second or B layer on top of the first or A layer. Naturally you put the spheres of the second layers in the hollows or dents of the first layer.

When you go for the third layer you have a choice. You can go for the option where the spheres of the third layer are in those hollows of the second layer that the third layer sits right on top of the first layer and thus is an A layer again.
Or you go for the other option where you produce a C- layer. We found that

- two kinds of stacking sequences both lead to a close-packed crystal:The stacking sequence **ABABABA...** produces an hexagonal crystal (hcp; hexagonal close packed)
- The stacking sequence **ABCABCA...** produces a cubic face-centered fcc crystal.



(a) Hexagonal close-packed (hcp)



(b) Cubic close-packed (ccp)

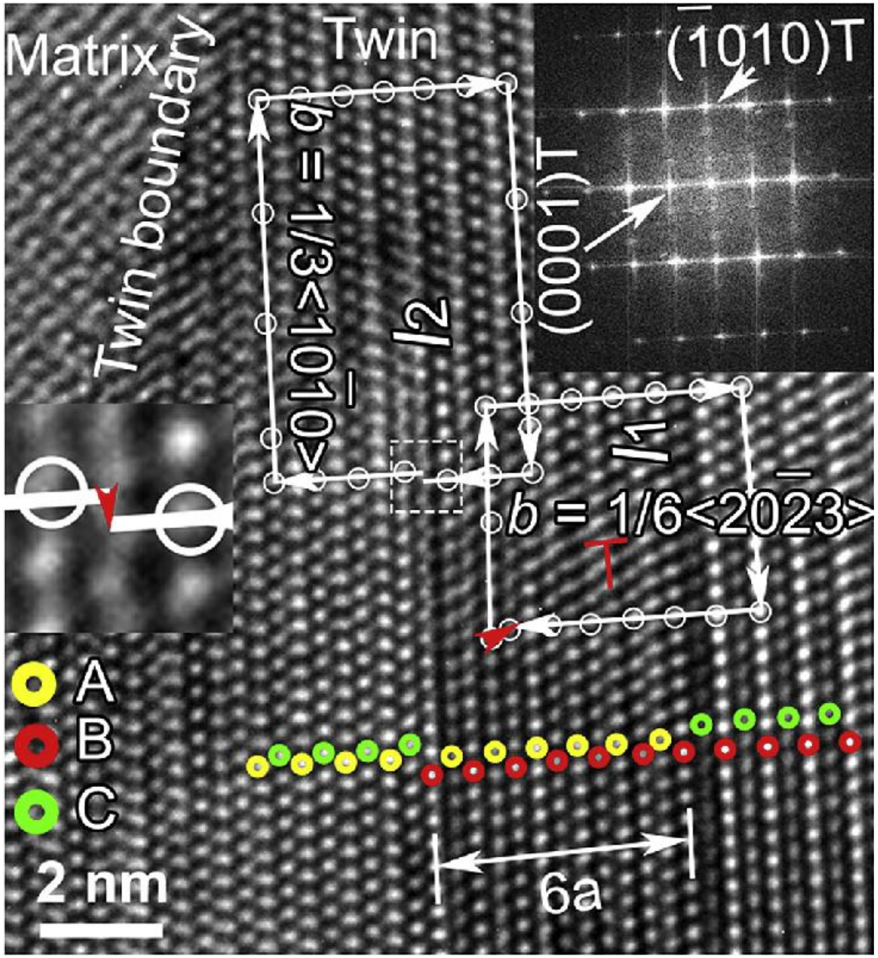


Fig. 7. HRTEM image showing the stacking faults in a {10 1}–{10 2} double twin (twin B marked in Fig. 4). The viewing direction is parallel to the vector CA shown in Fig. 2. Inserts are the FFT pattern from the twinned area, and the enlarged image of the square region surrounding by dash lines, respectively. The Burgers circuit and stacking sequence for I1 and I2 are indicated, and the Burgers vectors are shown by arrow heads.

S.Q. Zhu, Simon P. Ringer, On the role of twinning and stacking faults on the crystal plasticity and grain refinement in magnesium alloys, Acta Materialia, Volume 144, 2018, Pages 365-375, ISSN 1359-6454, https://doi.org/10.1016/j.actamat.2017.11.004.

Formation of Stacking Faults and the Screw Dislocation-Driven Growth: A Case Study of Aluminum Nitride Nanowires

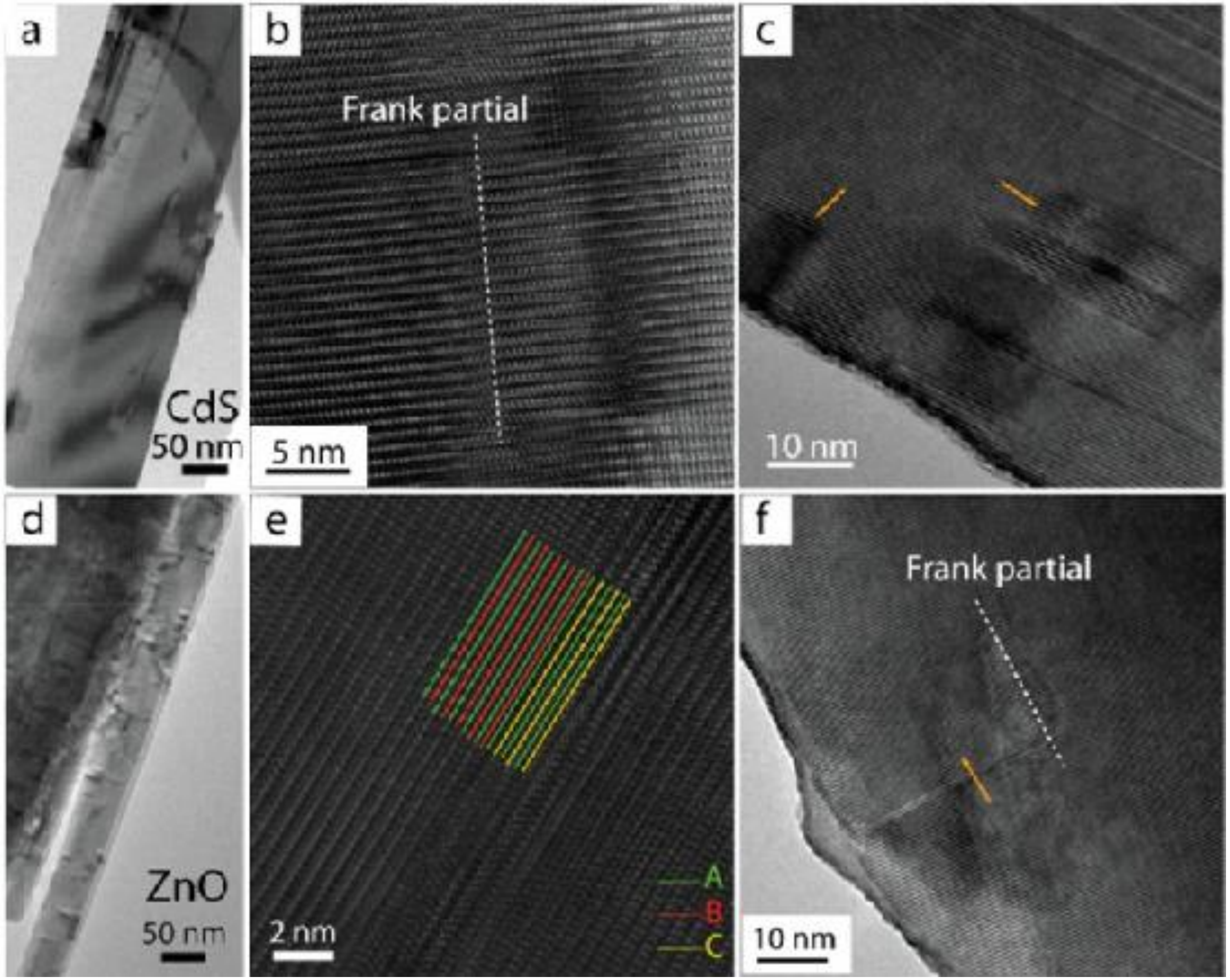


Figure 8. Type I stacking faults and Frank partial dislocations in CdS (a c) and ZnO (d f) NWs. (a) Low-resolution TEM image of a CdS NW containing zigzag-shaped stacking faults. (b) HRTEM image showing the faulted region in panel a with a Frank partial dislocation. (c) HRTEM image of a CdS NW containing closed-loop stacking faults. (d) Low-resolution TEM image of a ZnO NW containing closed-loop stacking faults. (e) HRTEM image showing the index of Type I stacking fault in the ZnO NW shown in panel d. (f) HRTEM image showing the Frank partial dislocation in a ZnO NW. Orange arrows indicate the faulted region.

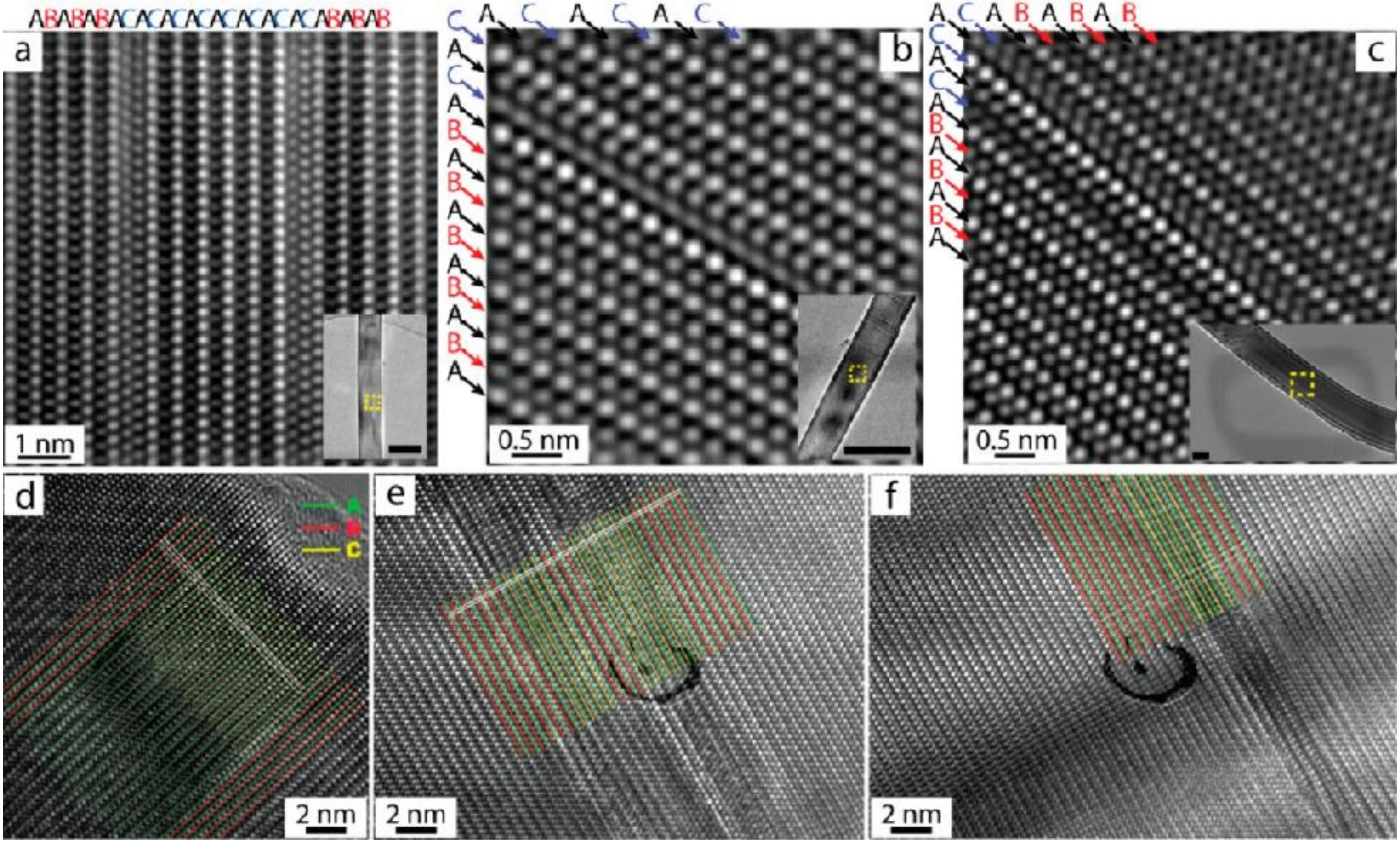
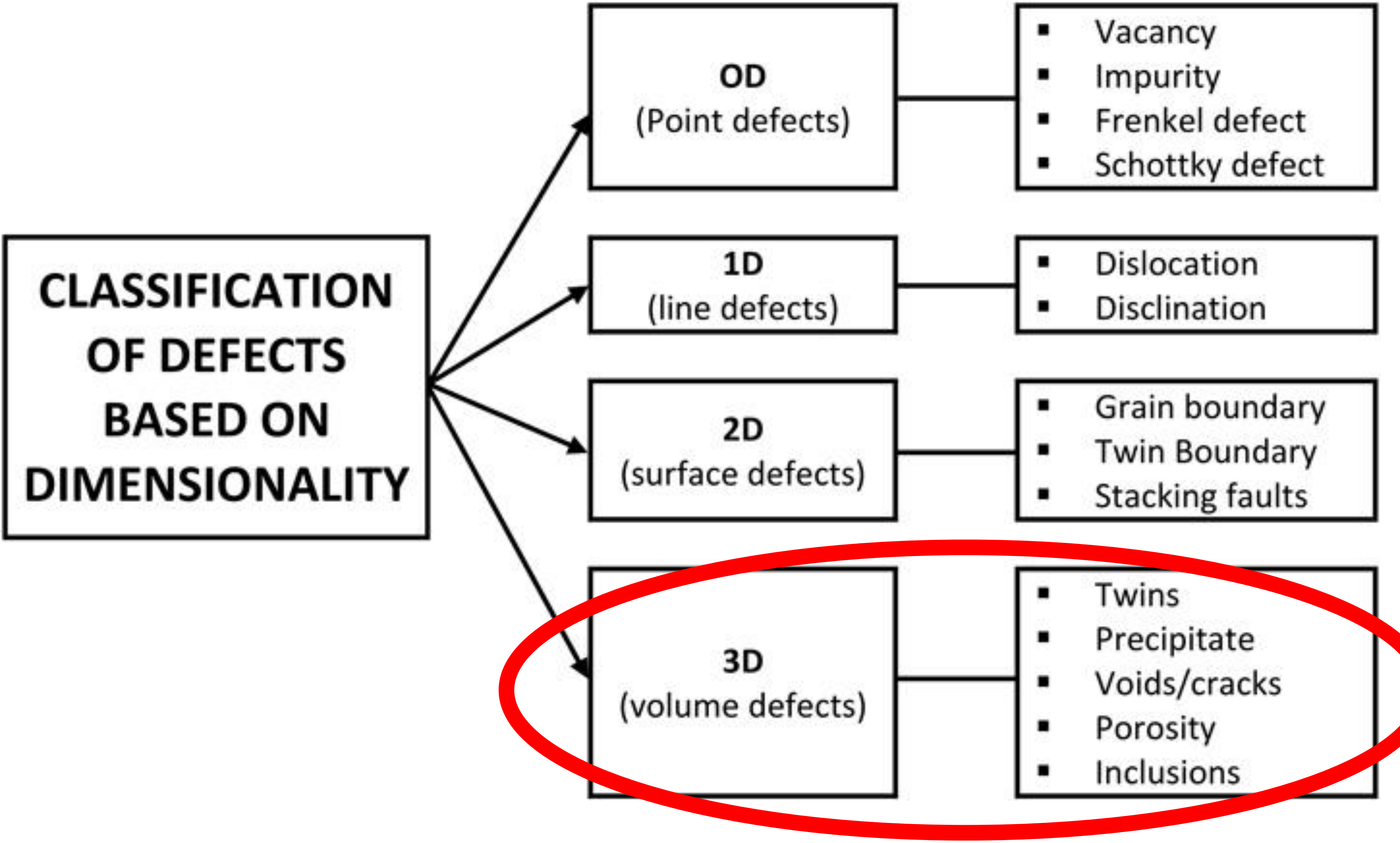


Figure 5. Identification of Type I stacking faults in the AlN NWs. The yellow dashed squared in the insets represent the region from which the HRTEM were acquired. All of the scale bars in the insets are 50 nm. Note that the circular features in panels e and f are due to a defect in the CCD camera of the TEM.

ts are next on our list.



CLASSIFICATION OF DEFECTS BASED ON DIMENSIONALITY

- **0D** (Point defects)
  - Vacancy
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  - Frenkel defect
  - Schottky defect
- **1D** (line defects)
  - Dislocation
  - Disclination
- **2D** (surface defects)
  - Grain boundary
  - Twin Boundary
  - Stacking faults
- **3D** (volume defects)
  - Twins
  - Precipitate
  - Voids/cracks
  - Porosity
  - Inclusions

BULK OR VOLUME DEFECTS

Bulk defects are also referred to as 3-dimensional defects

- Precipitates (impurities can cluster together to form small regions of a different phase).
- Pores
- Cracks
- Inclusions
- **Voids** — small regions where there are no atoms, and which can be thought of as clusters of vacancies

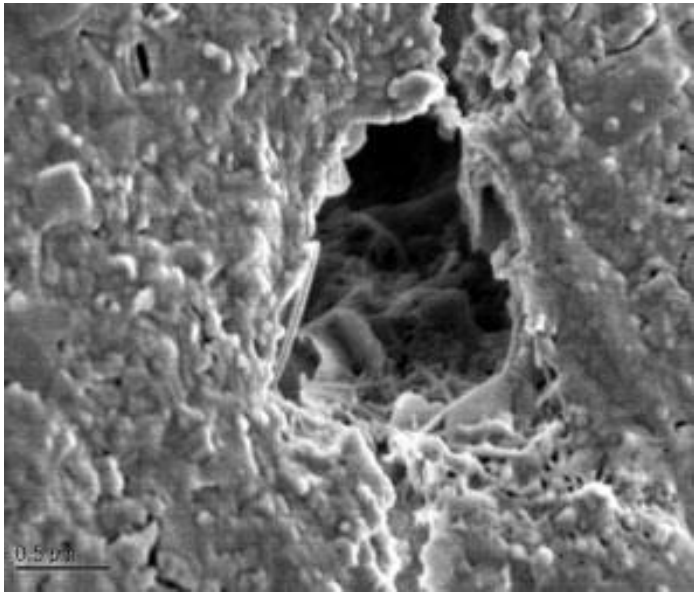
Much larger defects than the previous ones, usually introduced during processing and fabrication steps

Pores - can greatly affect optical, thermal, mechanical properties
Cracks - can greatly affect mechanical properties
Foreign inclusions - can greatly affect electrical, mechanical, optical properties

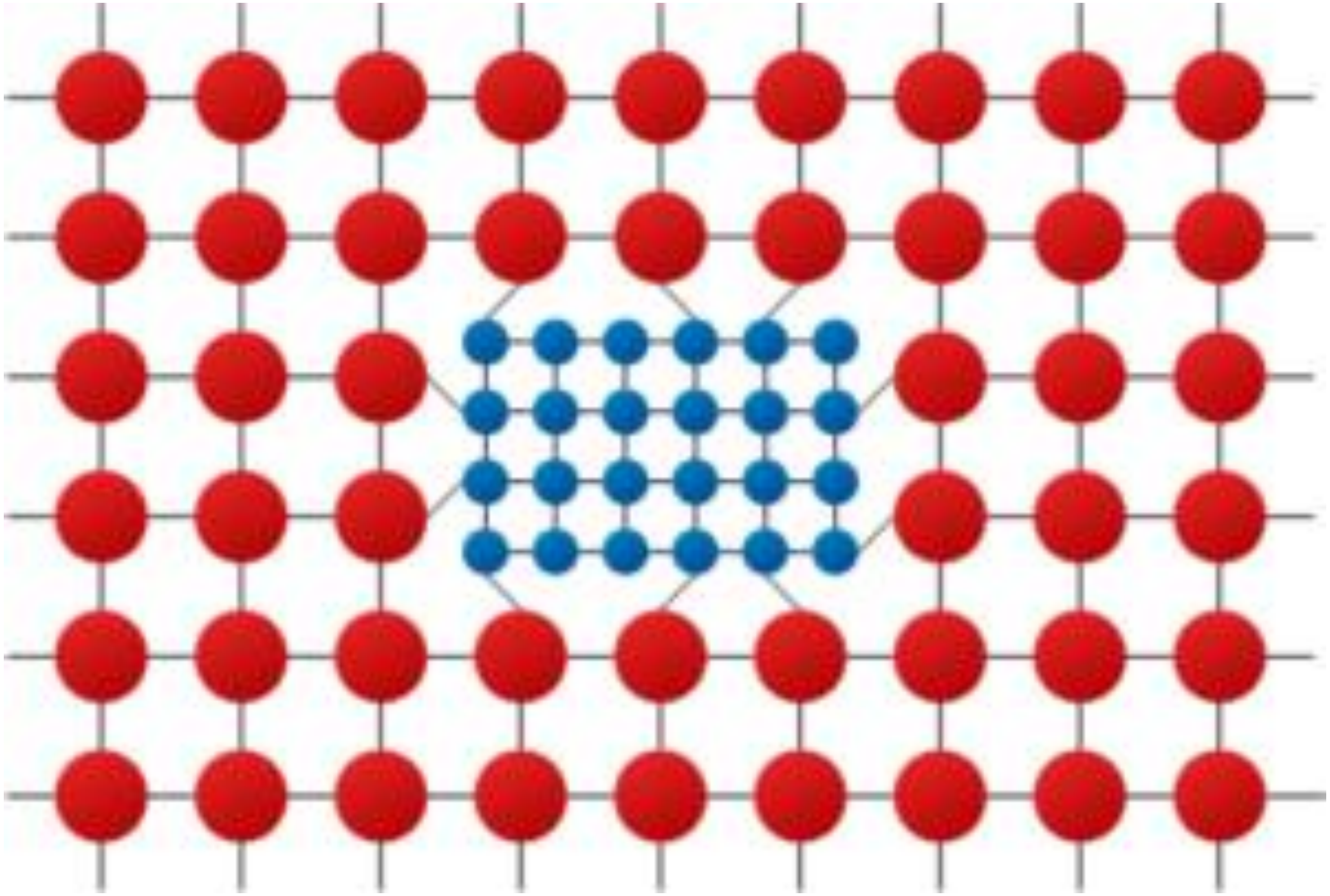
Bulk defects occur on a much bigger scale than the rest of the crystal defects discussed in this section. However, for the sake of completeness and since they do affect the movement of dislocations, a few of the more common bulk defects will be mentioned.

Voids are regions where there are a large number of atoms missing from the lattice.

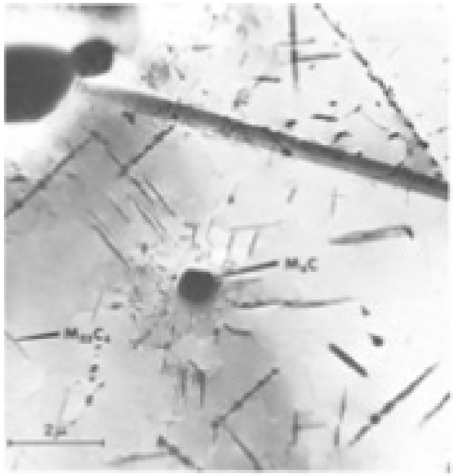
The image to the right is a void in a piece of metal The image was acquired using a Scanning Electron Microscope (SEM). Voids can occur for a number of reasons. When voids occur due to air bubbles becoming trapped when a material solidifies, it is commonly called porosity. When a void occurs due to the shrinkage of a material as it solidifies, it is called cavitation.



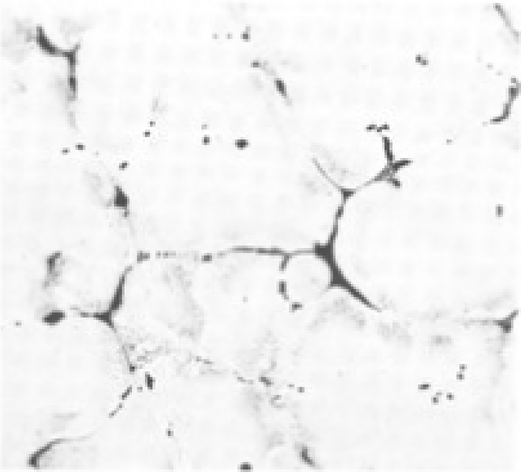
The so-called *precipitations* are an accumulation of chemical compounds (phases) in the metal. In addition to precipitations, pores or other inclusions are among the 3-dimensional defects.



Volume Defects



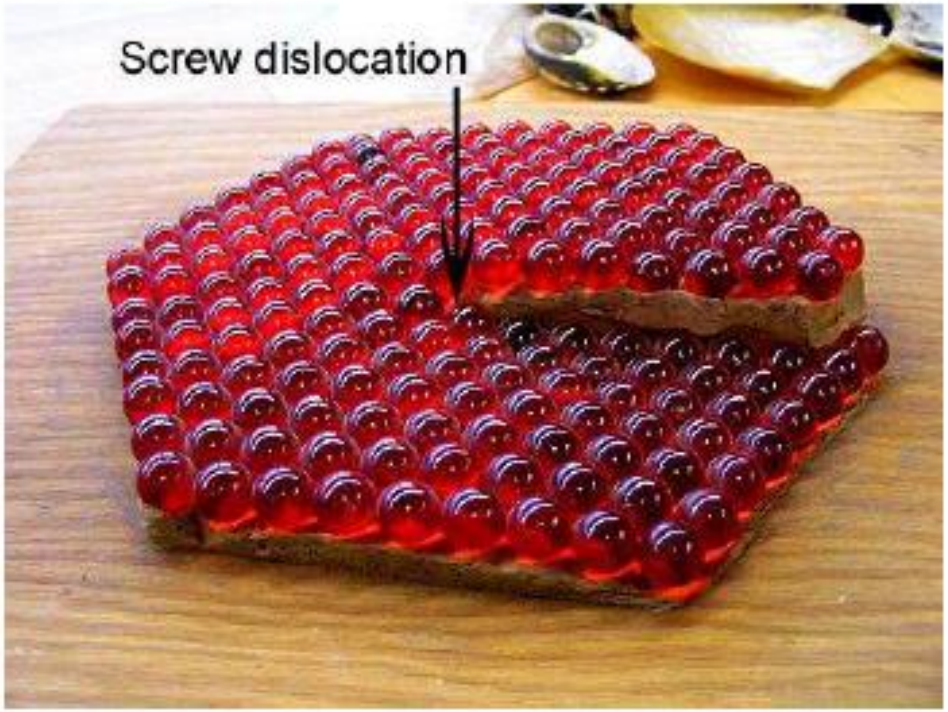
Inclusion

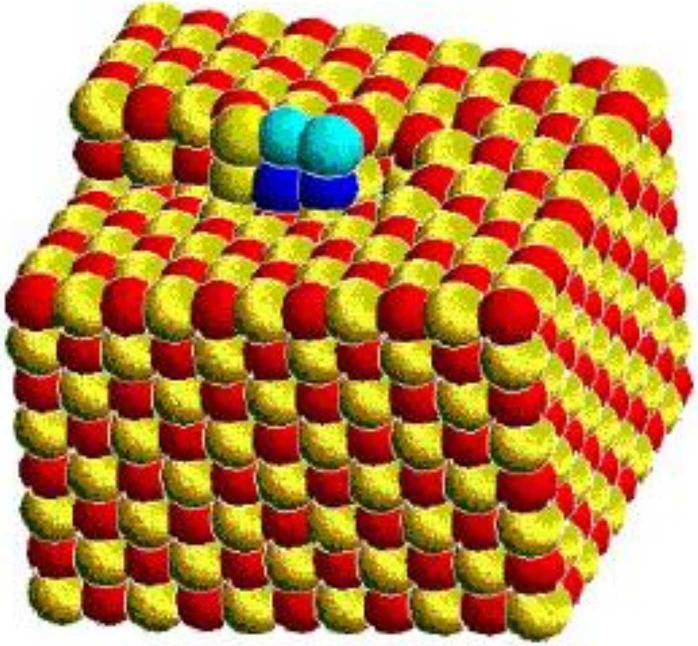


Voids/Pores

- Most common are second phases (e.g. salt in water)
- Cracks represent macroscopic volumetric defects

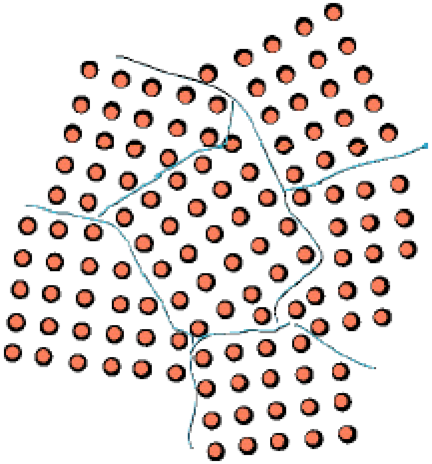
Another *linear* defect is a **screw dislocation.** This occurs when a stress is applied to the crystal and the dislocation of the line of atoms is perpendicular to the stress.





There are also planar defects such as grain boundaries. Chemical twinning (planar defects) contains unit cells mirrored about the twin plane through the crystal.

There are also *planar defects* such as **grain boundaries**.



Chemical twinning (*planar defects*) contains unit cells mirrored about the twin plane through the crystal.