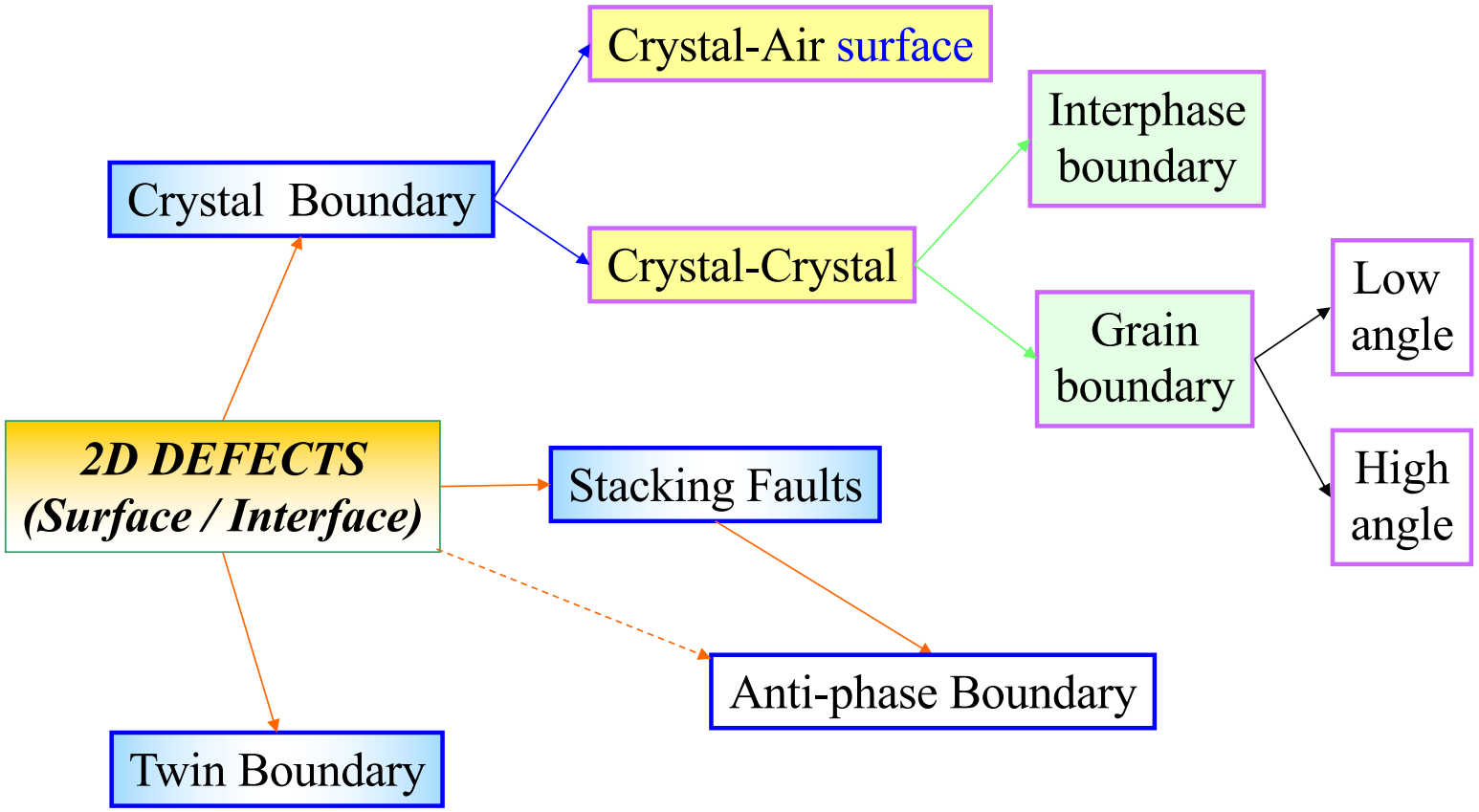
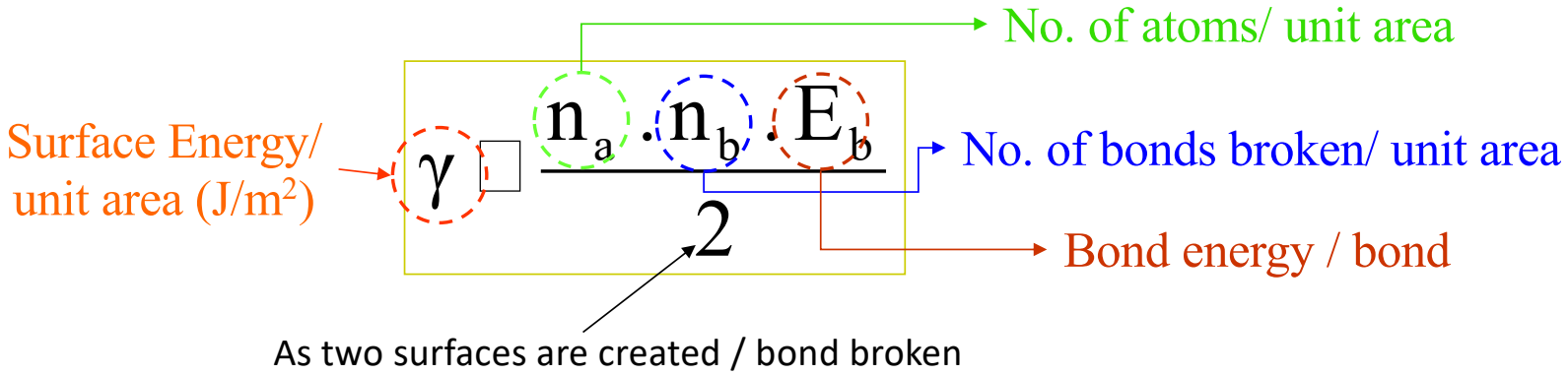

2D DEFECTS
(Surface / Interface)
Crystal Boundary
Crystal-Air surface
Crystal-Crystal
Interphase boundary
Grain boundary
Low angle
High angle
Stacking Faults
Anti-phase Boundary
Twin Boundary

Surface Imperfections

- 2D in a mathematical sense
- The region of distortion is ~ few atomic diameters in thickness

External surface of the crystal

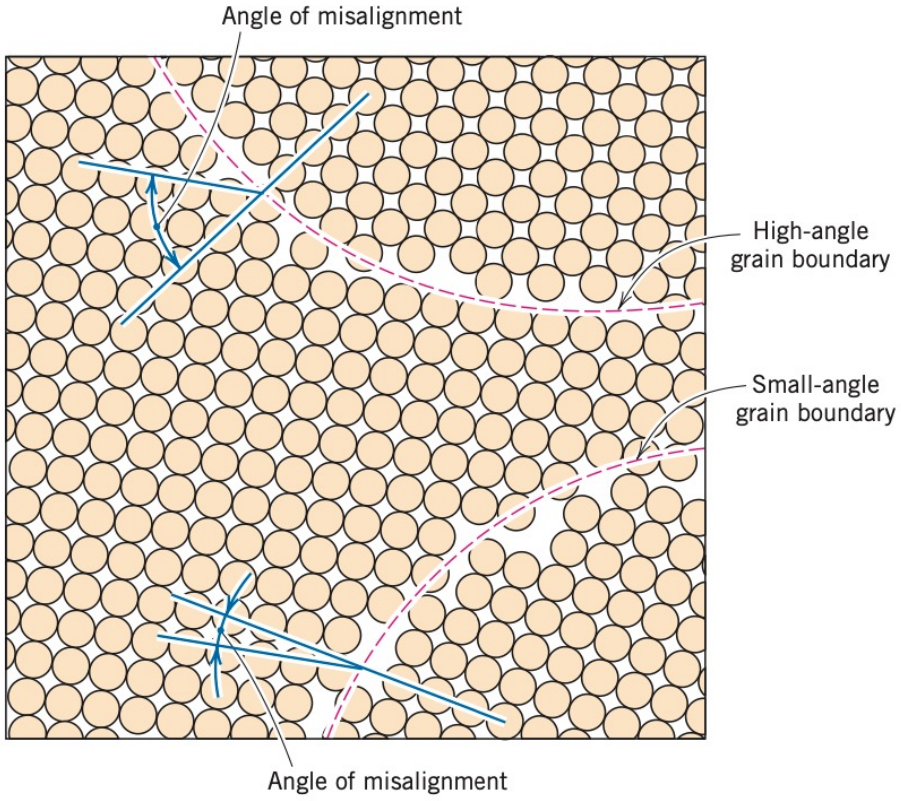
- External surfaces have energy related to the number of bonds broken at the surface

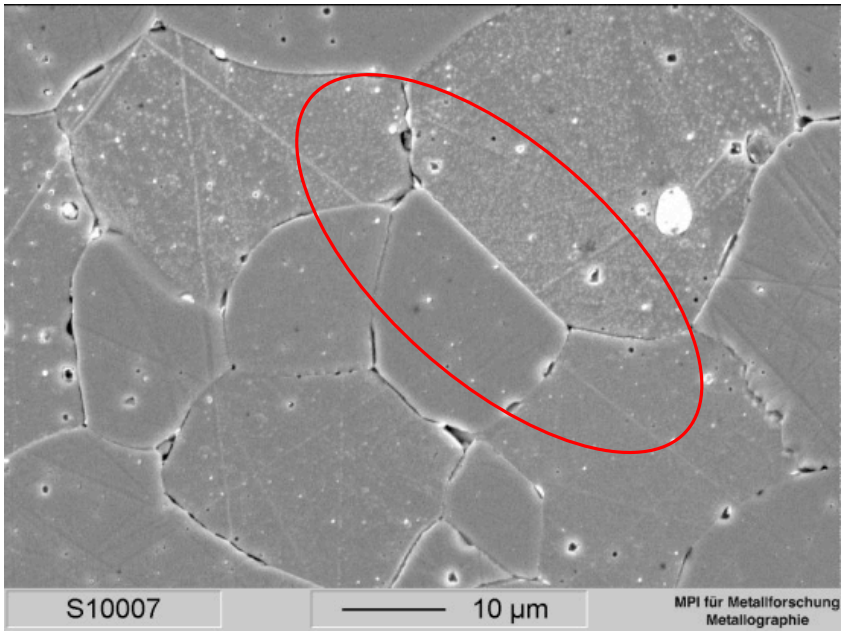


Surface free energies of some crystals (J/m^2)								
NaCl	LiF	CaF_2	MgO	Si	Ag	Fe	Au	Cu
0.30	0.34	0.45	1.2	1.24	1.14	1.4	1.4	1.65

Grain boundaries

Boundary between crystals having different crystallographic orientations in a polycrystalline material.





Grain boundaries in $SrTiO_3$

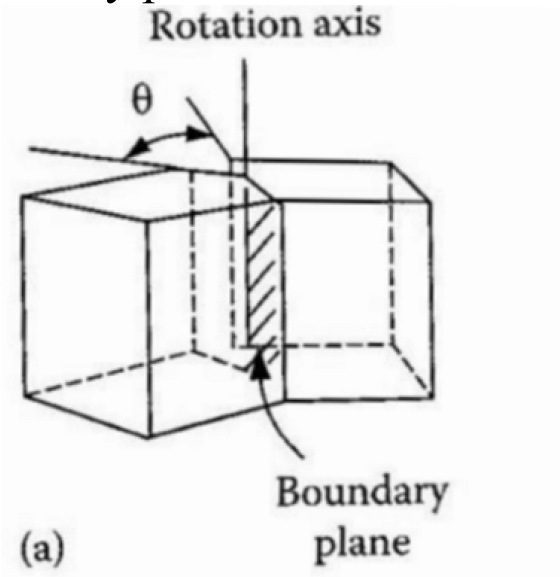
Low angle grain boundaries *(misorientation < 10°)*

Two extremes

TILT

An array of edge dislocations

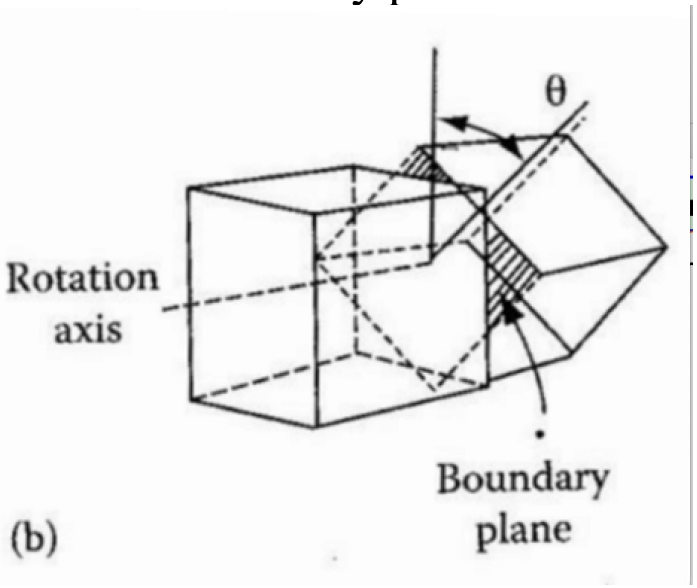
- Rotation axis lies on the boundary plane



TWIST

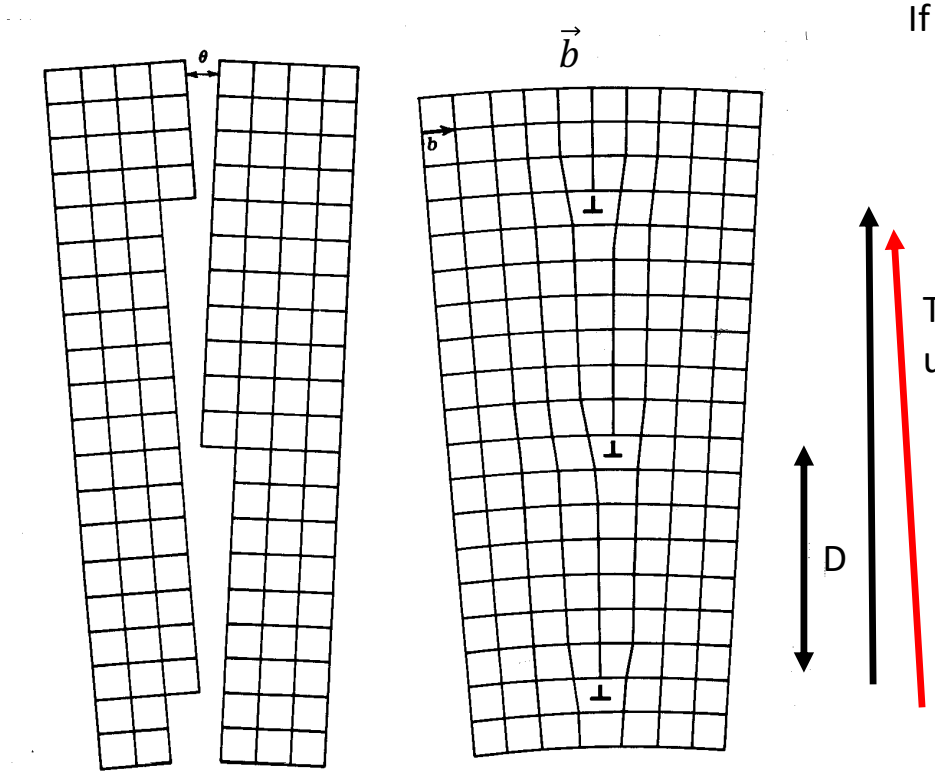
An array of screw dislocations

- Rotation axis lies ⊥ to the boundary plane



Tilt Qualifications

For a symmetric low angle grain boundary



If h is the total length of the crystal with the boundary

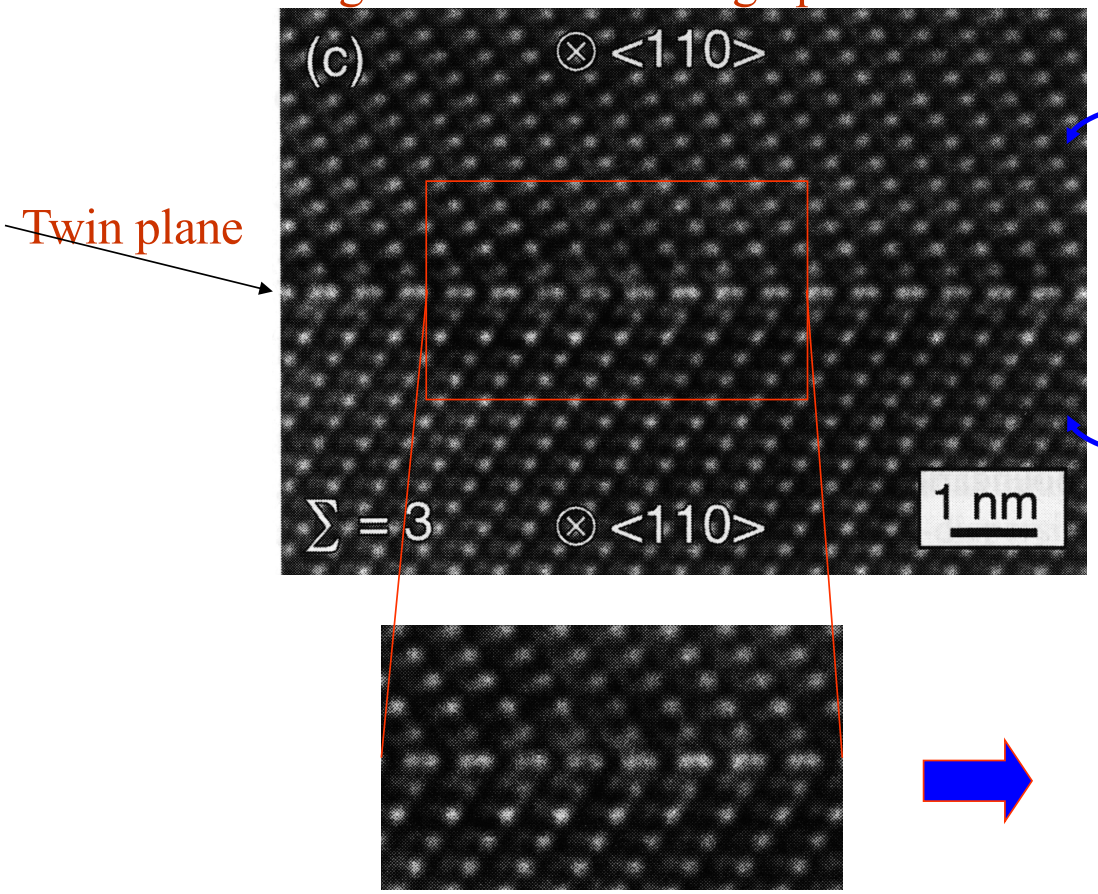
$$\frac{b}{2D} = \tan\frac{\theta}{2}$$

Then for small angles, total number of dislocations per unit length

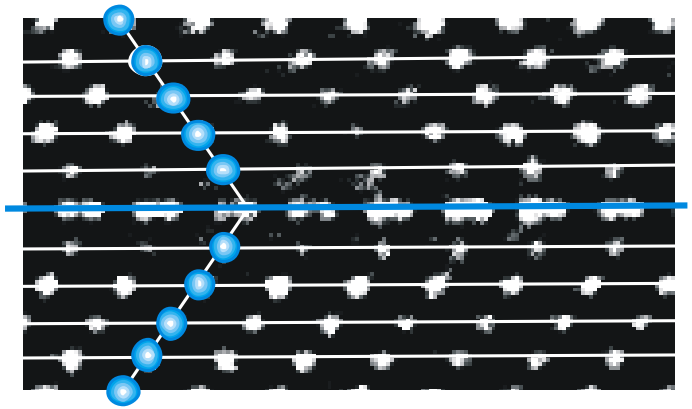
$$\frac{1}{D} \cong \frac{\theta}{b}$$

Twin boundary in Fe doped $SrTiO_3$ bicrystals *(artificially prepared)*

High-resolution micrograph



Mirror related variants

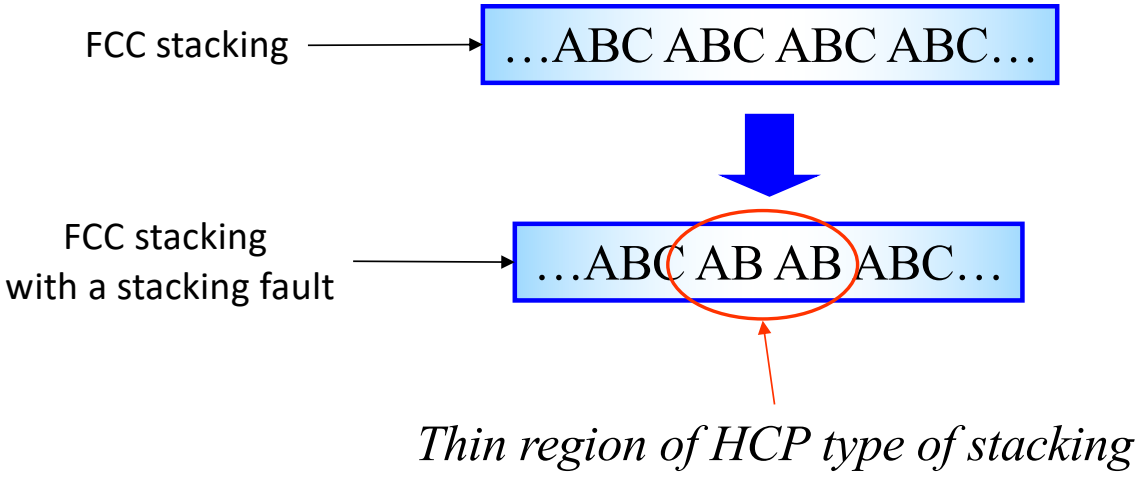


- The atomic arrangement on one side of the twin boundary is related to the other side by a symmetry operation (usually a mirror)
- Twin boundaries usually occur in pairs such that the orientation difference introduced by one is restored by the other
- The region between the regions is called the twinned region

[1] S. Hutt, O. Kienzle, F. Ernst and M. Rühle, Z Metallkd, **92** (2001) 2

Stacking Fault

- Error in the sequence of stacking atomic planes → Stacking fault
- Defined by a shift vector



- In above the number of nearest neighbours remains the same
  but next-nearest neighbours are different than that in FCC
- Stacking fault energy ~ 0.01 – 0.05 J/m^2
- Stacking fault in HCP can lead to thin region of FCC kind of stacking

Comparison of Energy of Various 2D Defects

Type of boundary	Energy (J/m^2)
Surface	~ 0.89
Grain boundary	~0.85
Twin Boundary	~ 0.63 0.498 (Cu)
Stacking Fault	0.08 (Cu) 0.2 (Al)

Comparison of Interfacial Energies of Various 2D Defects

Metal	Surface	Solid/ Liquid	Grain Boundary	Twin Boundary	Stacking Fault
	(J/m^2)				
Gold	1370	132	364	~10	55
Silver	1140	126	790	-	17
Platinum	1310	240	1000	196	~95
Nickel	1860	255	690	-	~400
Aluminium	1140	-	625	120	~200
Copper	1750	177	646	44	73
Iron	1950	204	780	190	-
Tin	680	54.5	-	-	-