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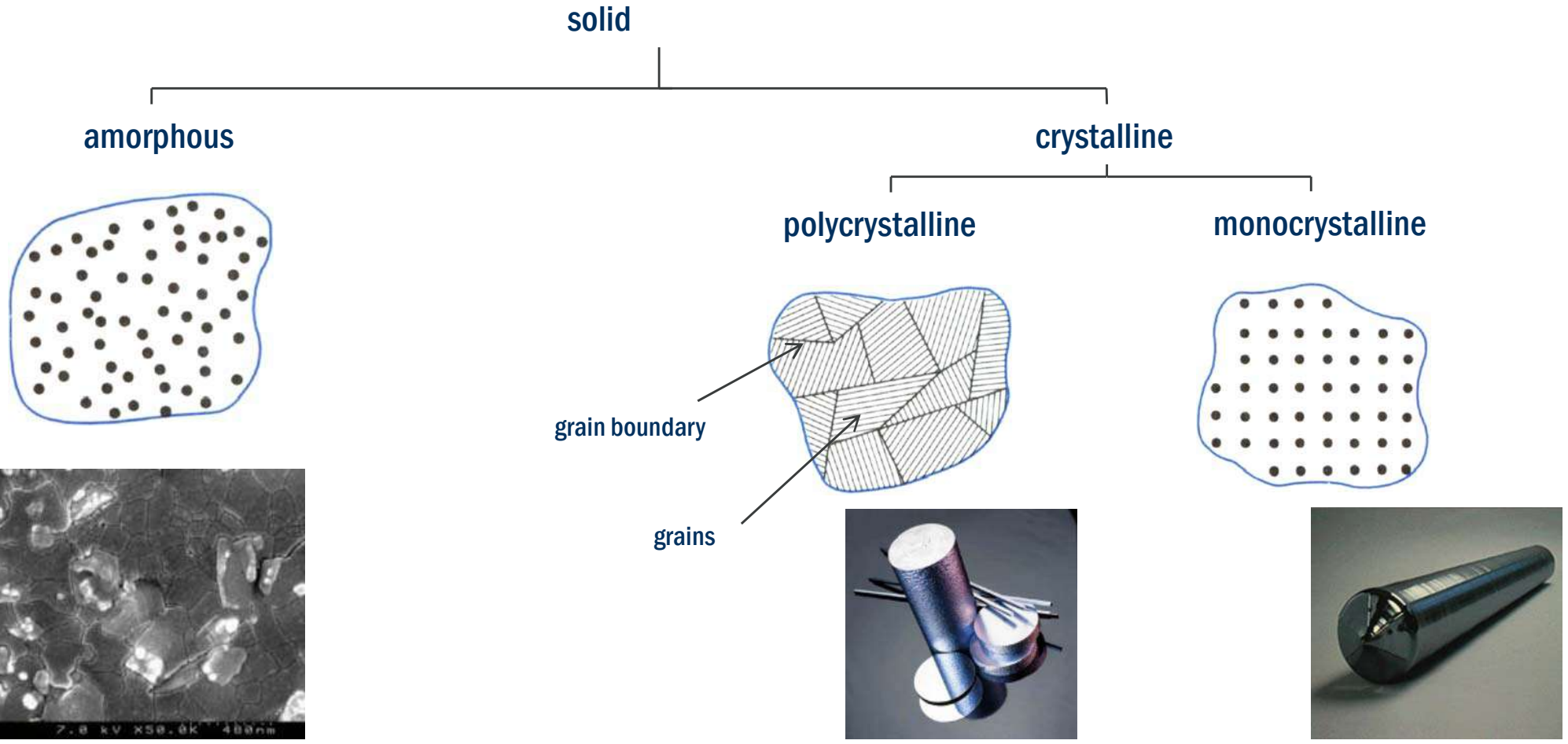
Microtechnologies
Chapter 2 – Wafer Fabrication

Dresden, 17.10.2024

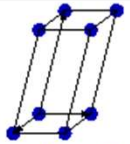
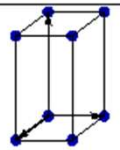
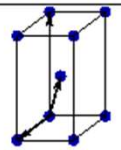
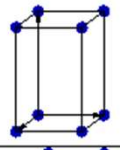
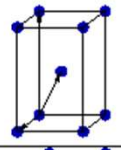
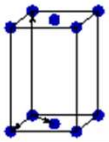
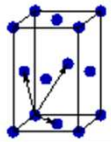
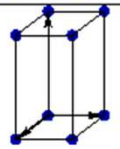
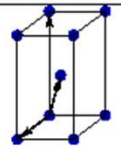
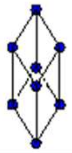
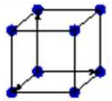
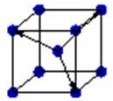
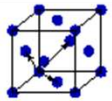
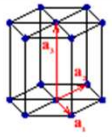
contents

contents

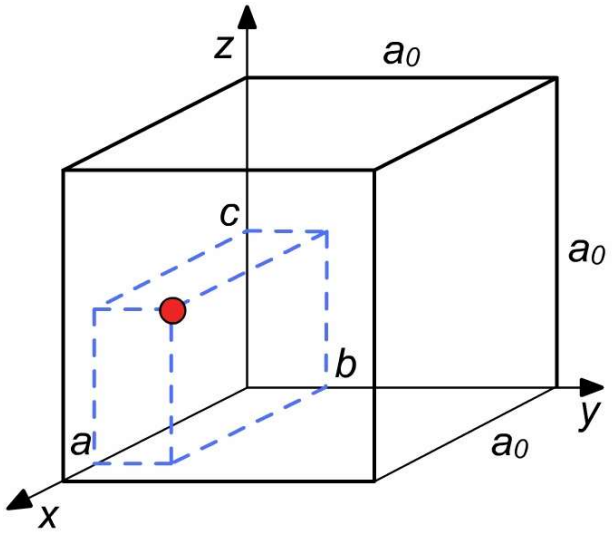
Solids are divided into amorphous and crystalline depending on their degree of crystallinity. Crystalline solids can be polycrystalline or monocrystalline.



Depending on the structure of the unit cell of the lattice, there are 14 Bravais lattices.

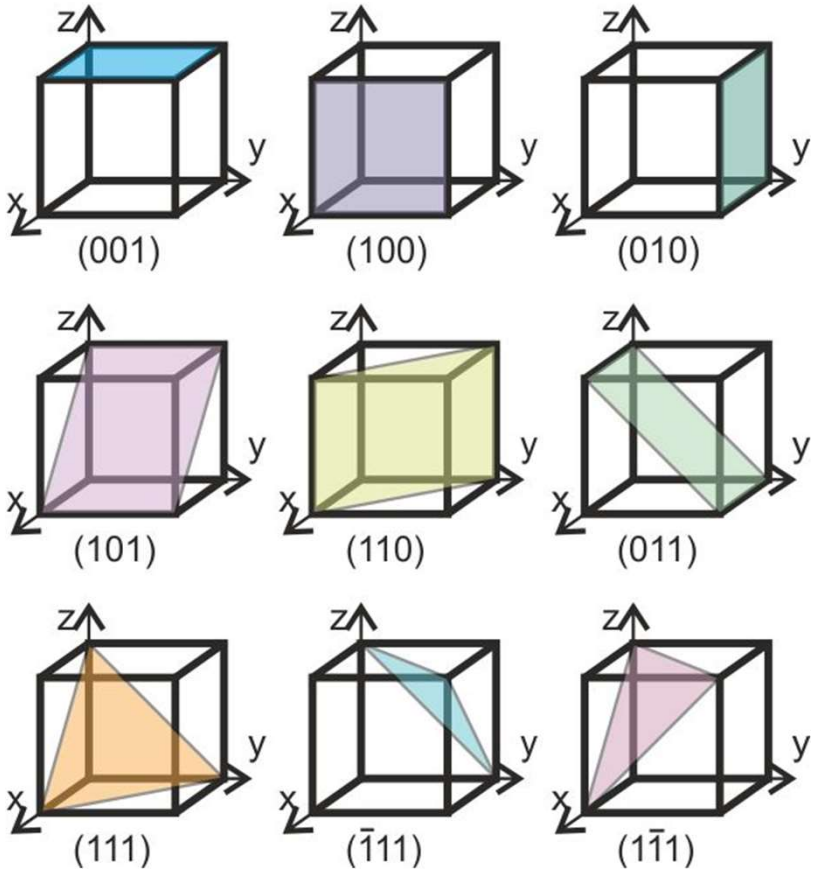
Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

Description of the atomic position in the EZ

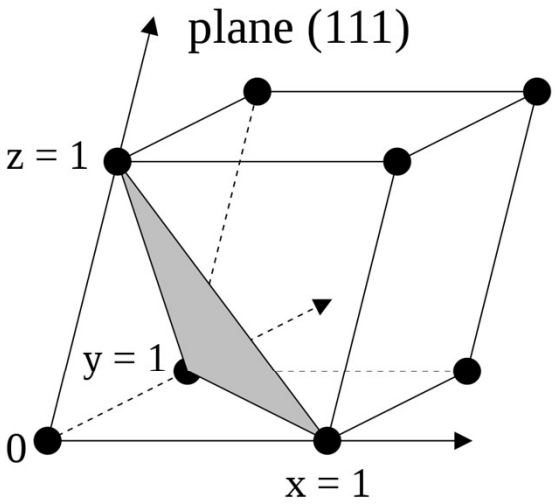


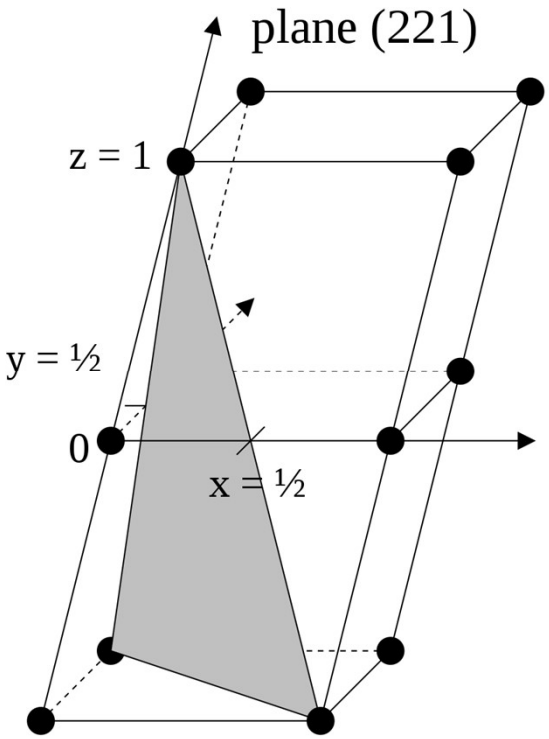
$$(a \cdot \mathbf{e}_x + b \cdot \mathbf{e}_y + c \cdot \mathbf{e}_z) \cdot a_0$$

Planes in a cubic primitive EZ



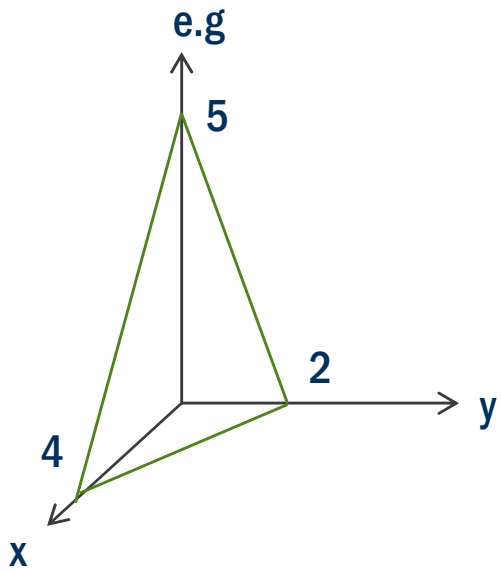
The indices of the planes are the **inverse** of the intersection points of the plane with the axes x, y and z, multiplied by the smallest common multiple of the denomintors (Aaaah!). These indices are called **Miller indices**, usually labelled (hkl). They are defined so that the plane intersects the endpoints of the vectors: (1/h)***x***, (1/k)***y***, (1/l)***z***





Example :

1. Determination of the intersection points with the axes: a=4, b=2 and c=5
2. Formation of the reciprocal values: 1/4, 1/2, 1/5,
3. Denominator determiner: here 20 → 5/20, 10/20, 4/20
4. Cross out the main denominator: 5, 10, 4
5. Miller indices: (hkl) = (5 10 4)

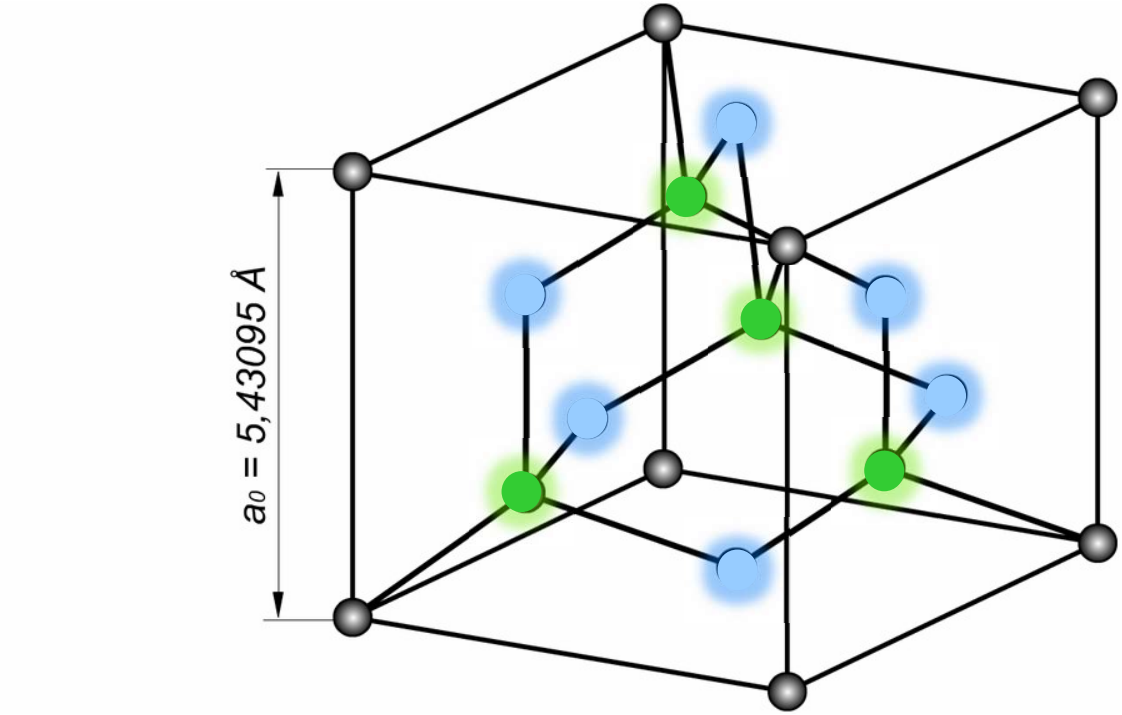


Describing planes and directions using Miller indices:

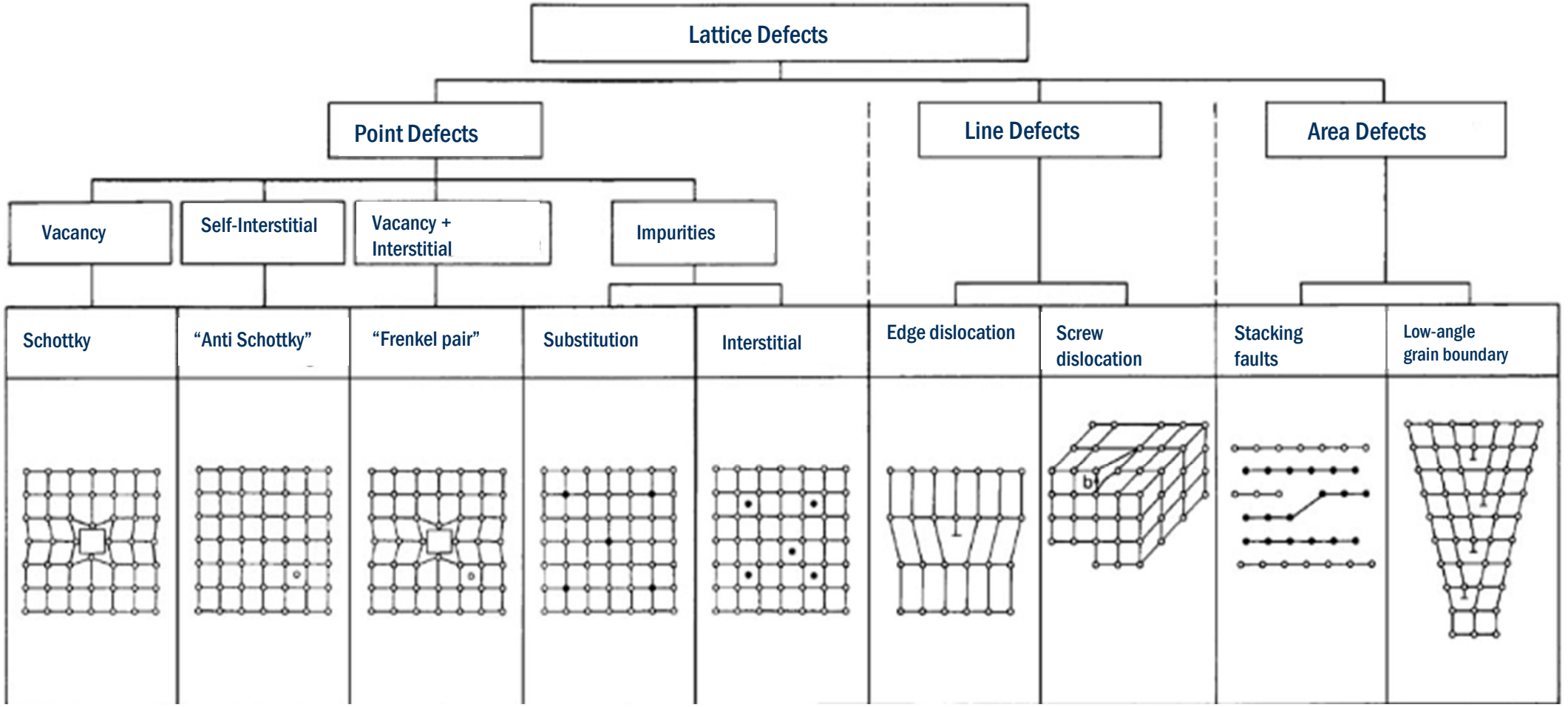
- Level: (hkl)
- Direction: [hkl]
- family of planes: { hkl }
- Group of directions: < hkl >

The crystal structure of the silicon unit cell corresponds to the diamond lattice. This consists of a face-centered cubic lattice and the basis {(0, 0, 0), (¼, ¼, ¼)}. This structure can be described as the combination of two nested face-centered cubic lattices that are shifted by ¼ of the space diagonal relative to each other.

Unit cell of the silicon diamond lattice



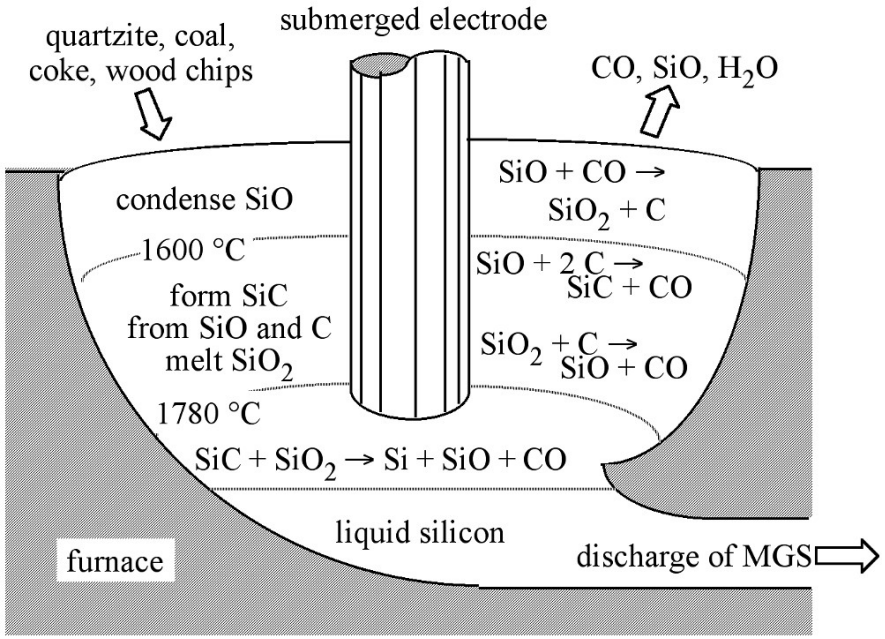
Any irregularity in an otherwise periodic crystal lattice is referred to as a lattice defect. They are differentiated according to their spatial extent - there are point errors, line errors and area errors.



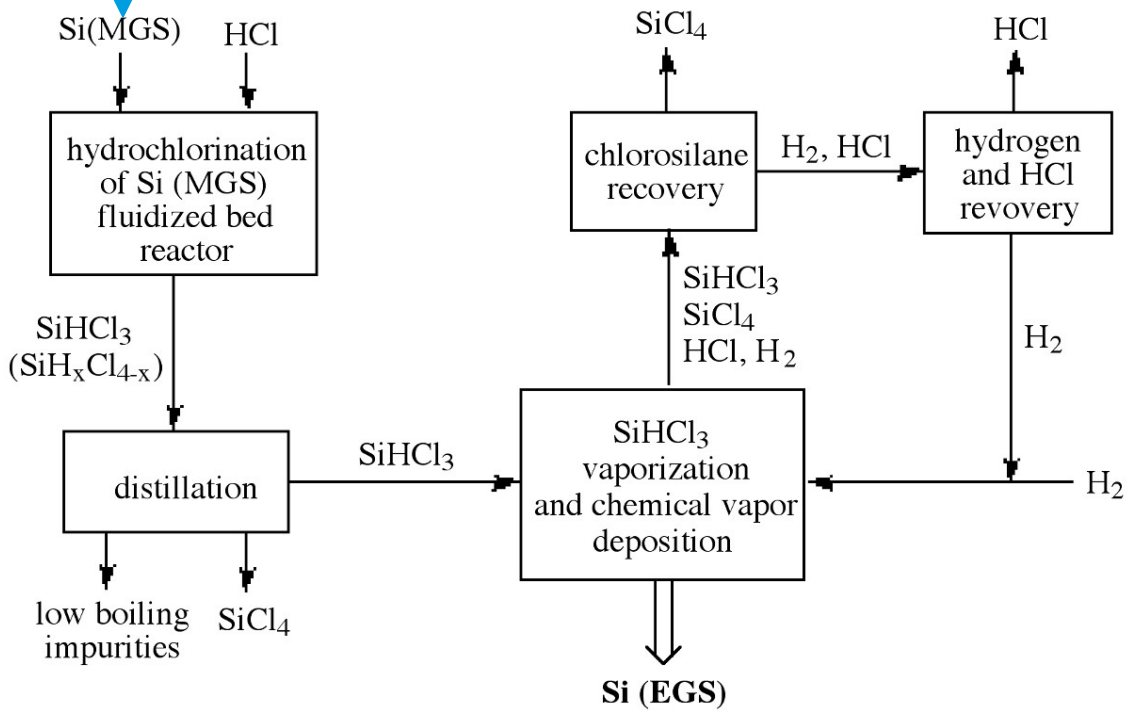
2.2 Crystal Groth – Overview –

Metallurgical-grade silicon (MGS)

$$SiO_2(liquid) + 2\,C(solid) \rightarrow Si(liquid) + 2\,CO(gas)$$



Electronic-grade silicon (EGS)



Single Crystal Production

Single Crystalline Si Ingots

Quartz is reduced using carbon in an arc furnace at 1500..2000 °C:

$$SiO_2 + 2C \rightarrow Si + 2CO$$

The resulting silicon has a purity of 98...99%. Less than 1% of the metallurgical Si produced is reused for the semiconductor industry. The majority is used for Al alloys, silicone resins and the steel industry.

Metallurgical silicon

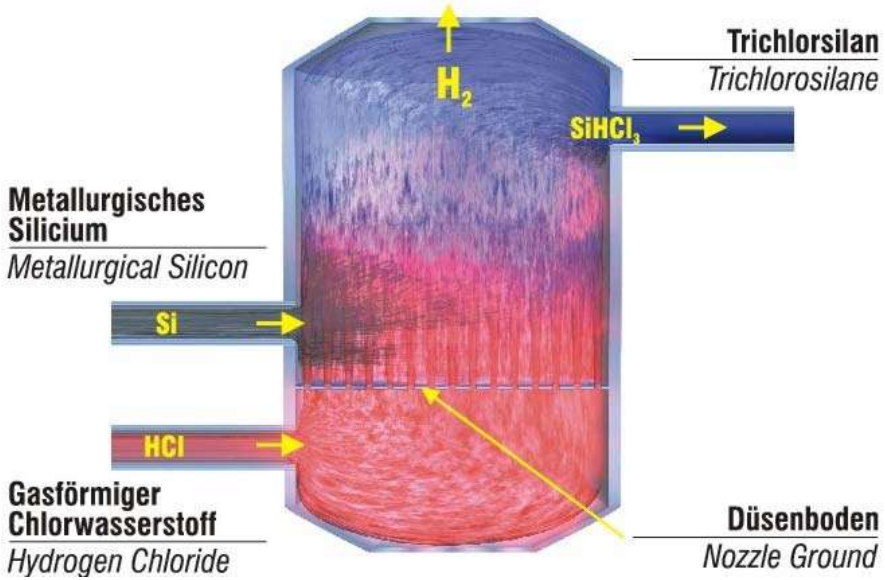
"Siemens process" – Part I: Triclorosilane Production

In the fluidized bed reactor, powdery metallurgical Si is converted to Trichlorosilane using gaseous HCl:

$$Si + 3HCl \rightarrow SiHCl_3 + H_2 \ (T \sim 350°C)$$

Impurities are removed by formation of their volatile chlorides, eg $FeCl_3$, $AlCl_3$, BCl_3 . The maximum concentration of your electrically active impurities achieved in this way is < 2 ppb. Further purification is done by standard distillation.

Fluidized bed reactor principle

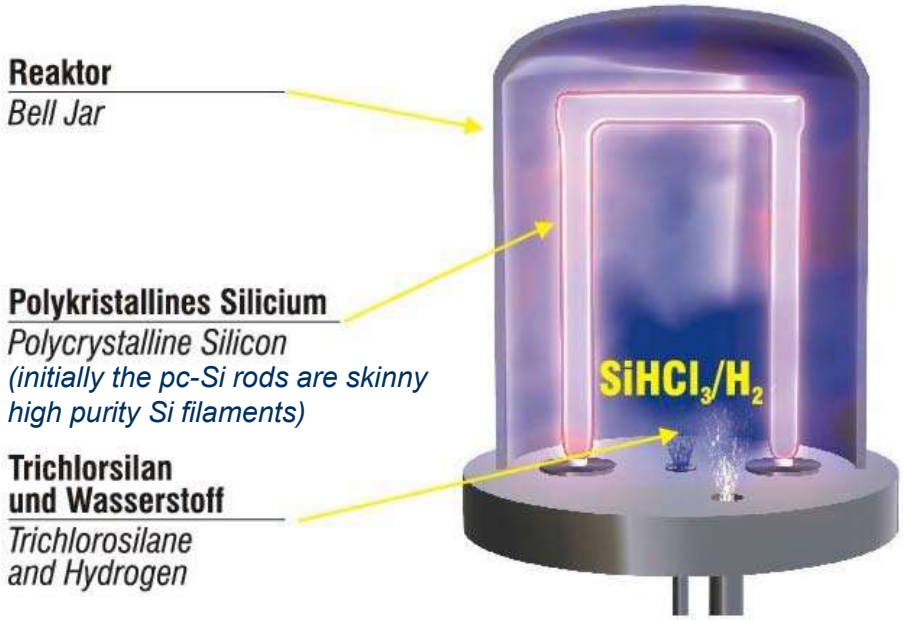


"Siemens process" – Part II: Polysilicon generation

Through pyrolytic decomposition of trichlorosilane, and deposition of high-purity poly-silicon on resistively-heated silicon filaments that grow into poly-silicon rods:

$$SiHCl_3 + H_2 \rightarrow Si + 3HCl\ (T = 1100\ °C, t = 200 \ldots 300\ h)$$

Production of a polycrystalline Si rod by pyrolytic decomposition

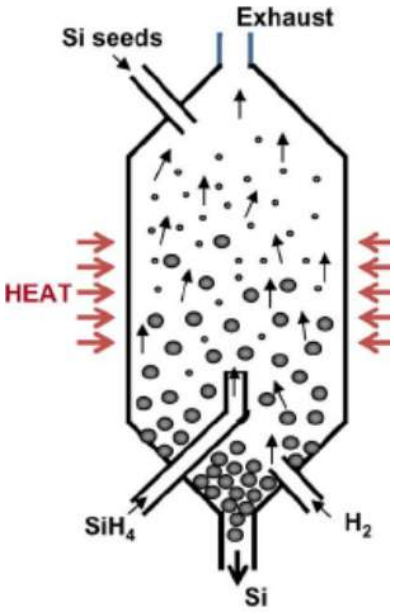


2.2 Crystal growth - purification to Electronic Grade Silicon (EGS) -

"Silane process"

This process produces silane (SiH_4) by reaction of Si with Mg:

$$Si + 2Mg \rightarrow Mg_2Si \; (T = 500\,°C)$$
$$Mg_2Si + 4\,NH_4Cl \rightarrow SiH_4 + 2\,MgCl_2 + 5\,NH_3 \; (T < 0\,°C)$$



Polycrystalline Si is obtained through pyrolytic decomposition of silane at 700...800 °C, similar to the Siemens process

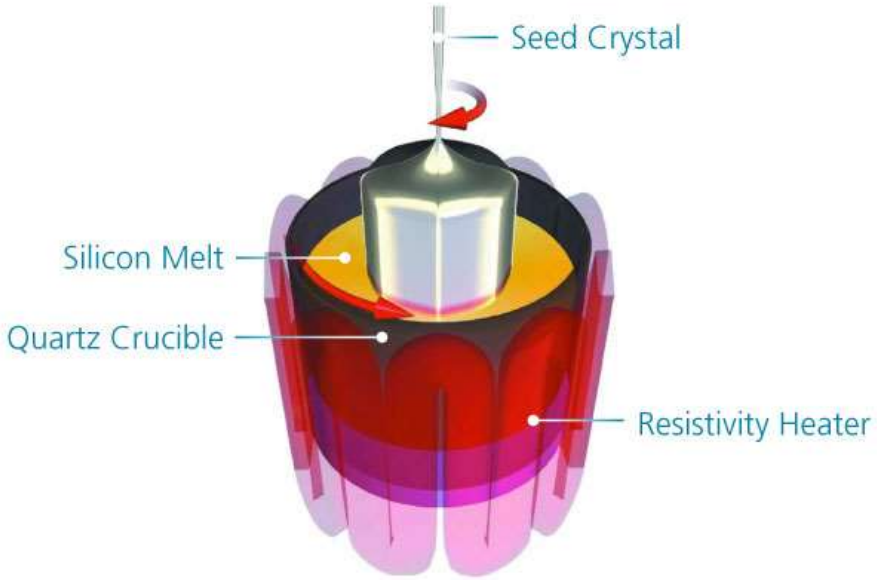
Advantages :
- higher purity (0.01...0.02 ppb)
- lower deposition temperature

Disadvantages :
- production of silane is expensive
- process engineering problems in the decomposition of silane

Czochralski (CZ) method

A seed crystal of the to growing material (monocrystalline Si) is submersed in the crystallizing substance (poly-silicon) a few degrees above to the melting point. By slow rotation and withdrawal, the solidifying material grows with the same crystal lattice as the seed crystal → single crystal.
The process is usually performed in an inert atmosphere, e.g. argon gas.

Scheme of the CZ process



Silicon single crystal for wafer production

2.2 Crystal growth - single crystal production -

Czochralski (CZ) method : Impurities after crystal growth

- Oxygen O
- Carbon C
- Electric active / inactive impurities

Typical concentrations of other impurities in CZ silicon (in ppb):

Ag	As	Au	Cd	Cl	Cr	Cu	Fe
<0,008	0,015	<10-5	0,008	-	<0,03	0,01	<0,1
Ga	In	K	Mn	Mo	Na	Ni	Pt
<0,002	<0,03	<0,3	<1	<0,03	0,03	<0,2	0,01
Sb	Se	Sn	Sr	Ta	W	Zn	Zr
0,002	<0,01	<0,3	<0,5	<0,001	<0,001	<0,05	<1

Czochralski (CZ) method: Impurities after crystal growth

- Oxygen O
    - Origin: Contact of the melt with the crucible wall
    - Concentration: 10^{17} to 10^{18} cm^{-3}
    - Part is built into the crystal and leads to precipitation of oxygen (SiO_2 -precipitates)

- Effects
    - Reduction of the charge carrier lifetime, mobility
    - Internal gettering of impurities

Czochralski (CZ) method: Impurities after crystal growth

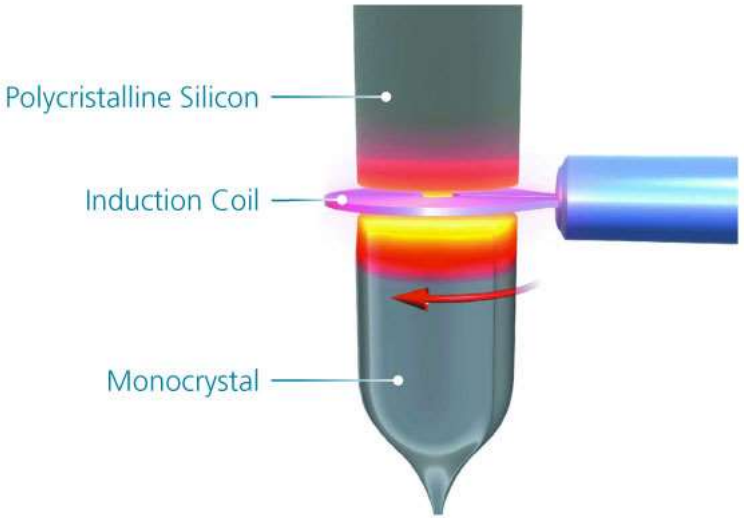
- Carbon C
    - Origin: CO and CO_2 enter the melt from the graphite crucible holder and graphite heater
    - Concentration: 10^{15} to 10^{17} cm^{-3}
    - Impact: crystal defects that can lead to device malfunctions
- Electrically active impurities
    - Donors (As, Sb, P)
    - Acceptors (B, Al, Ga, In)
    - Traps in the middle of the band gap (e.g. Au, Fe, Cu)
    - Effect: Reduced charge carrier lifetime
- Electrically inactive impurities
    - precipitates
    - mechanical interference → indirect electrical interference

Crucible-free zone drawing - Float Zone (FZ) process

A rotating poly-Si feed rod is melted at the end by induction heating in a narrow zone, and brought into contact with a seed crystal. As the rod slowly rotates, the melt zone is slowly moved up the poly-silicon rod - the solidifying melt grows with the same crystal structure as the seed.
The process is usually performed in an inert atmosphere, e.g. argon gas.

Impurities accumulate in the melting zone and eventually attach to the top end of the feed rod, which is removed after cooling.

Schematic of the FC procedure



Grown Si crystal

How are the (intentional) dopants added?

- **CZ method**: directly added to the crucible (e.g. B, As, P, Sb)

- **FZ process**: blowing onto the melting zone with a gaseous compound of the dopant (e.g. B_2H_6, PH_3, SbH_3, AsH_3)

Dopants in the crystal - Segregation

Some trace impurities always exist in the crystal. How big this portion is, can be calculated from the corresponding *segregation coefficients k:*

$$k = \frac{C_{cr}}{C_m}$$

C_{Cr}: Concentration of the foreign atom in the crystal
C_m: Concentration of the foreign atom in the melt

The smaller k is, the purer becomes the crystal .

Segregation coefficient k of different elements in silicon

Li	Cu	Ag	Au	Zn	Cd	Fe
0,01	$4 \cdot 10^{-4}$	$1 \cdot 10^{-6}$	$2{,}5 \cdot 10^{-5}$	$1 \cdot 10^{-5}$	$1 \cdot 10^{-6}$	$8 \cdot 10^{-6}$
B	Al	Ga	In	Tl	C	Co
0,8	$2 \cdot 10^{-3}$	$8 \cdot 10^{-3}$	$4 \cdot 10^{-4}$	$1{,}7 \cdot 10^{-4}$	0,07	$8 \cdot 10^{-6}$
Sb	Bi	O	S	Cr	Mn	Ta
0,023	$7 \cdot 10^{-4}$	1,4	$1 \cdot 10^{-5}$	$1{,}1 \cdot 10^{-5}$	$1 \cdot 10^{-5}$	$1 \cdot 10^{-7}$
As	P					
0,3	0,35					

Problems:

- Boron (k=0.8) => low-doped crystals are p-type
- Oxygen (k=1.4) => enrichment of oxygen in the crystal phase

Addition of dopants - Dopant distribution

The enrichment of dopants in the melt with progressive crystal growth can be calculated, accounting for segregation and melt reduction :

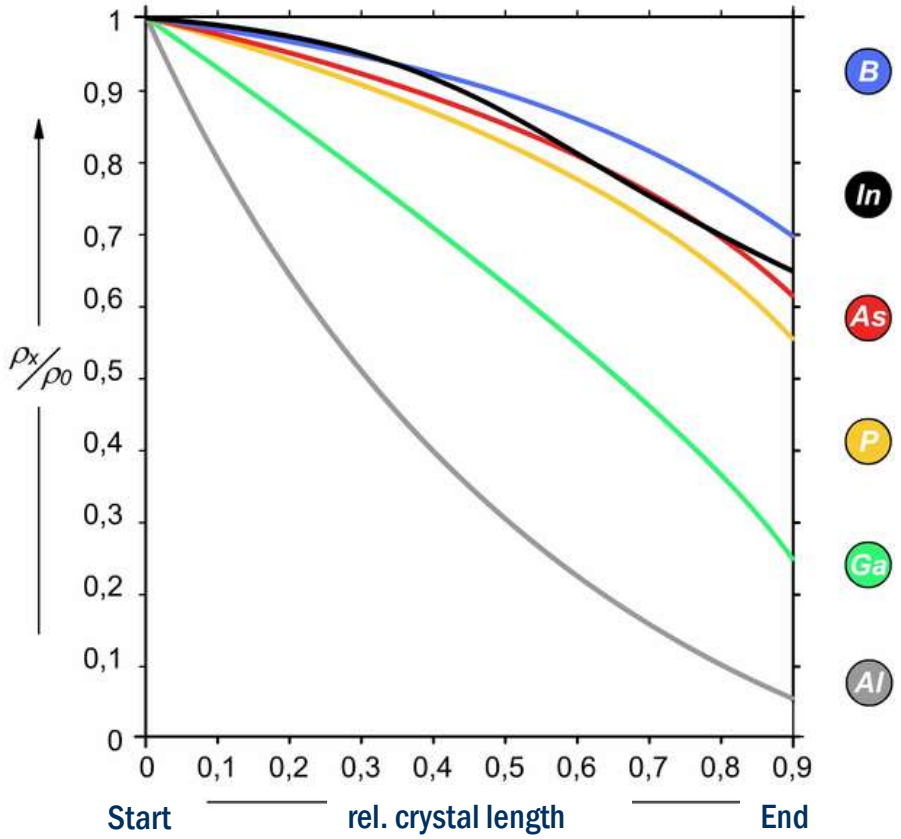
$$c = c_0 \cdot k \cdot (1 - g)^{k-1}$$

c: dopant concentration in the crystal at the solidification front
g: fraction of the original melt volume that has solidified
c_0: original dopant concentration in the melt

Addition of dopants - dopant distribution

Due to segregation of dopants, the specific resistance of the growing crystal is *not constant*!

Axial resistance change of CZ crystals for different dopants

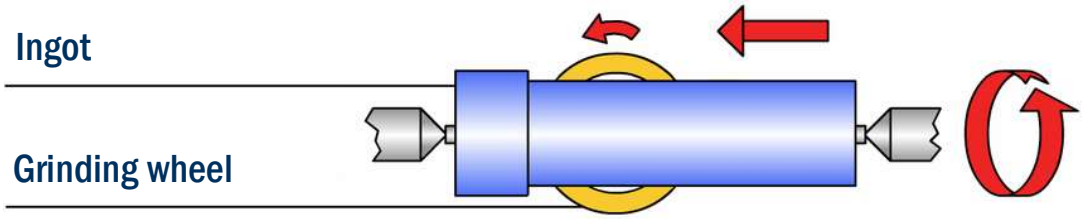


Process steps from ingot to wafer

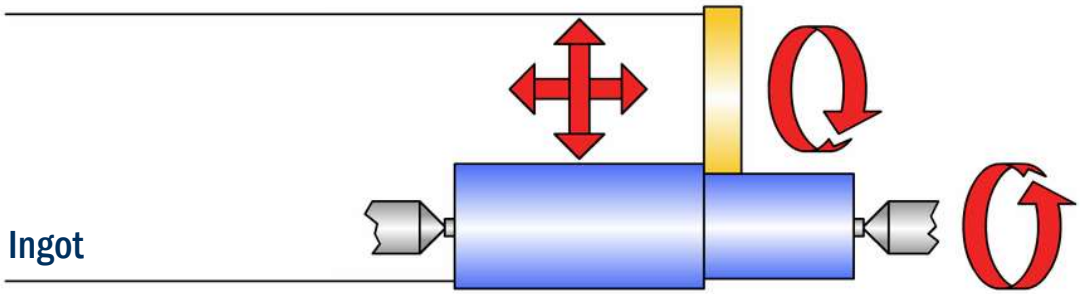
Process Step	Material Loss
Cutting off ends of the ingot	10-30 %
Grinding to desired diameter	5%
Orientation notches	1%
Cleaning etch	
Sawing	300-500 μm/disc
Lapping	10-50 μm/disc
Rounding/Bevelling	
Etching	15-80 μm/disc
Polishing	20-50 μm/disc

First, silicon monocrystal is ground to a round shape, down to the desired diameter

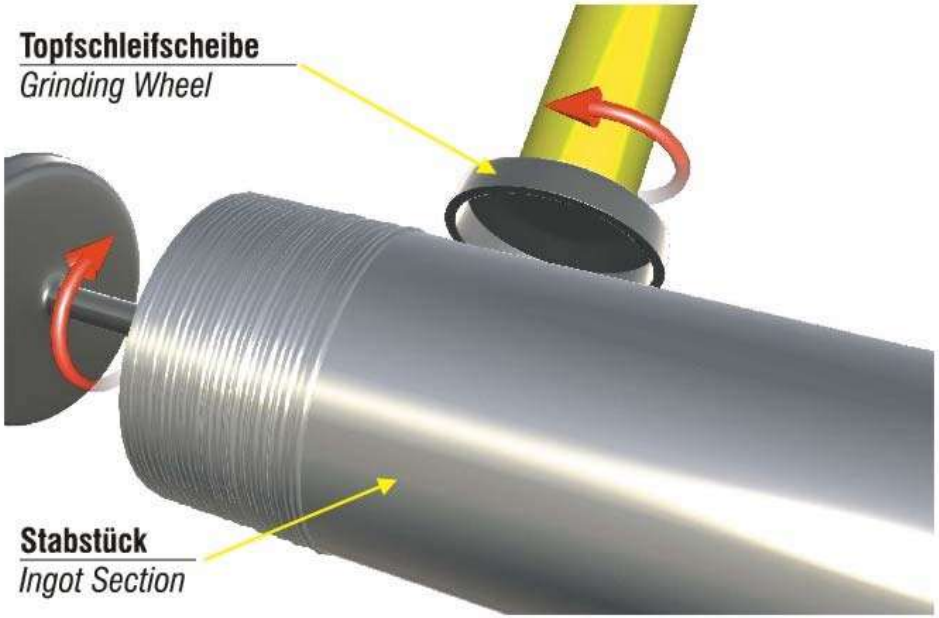
Top Griding



Lathe Grinding

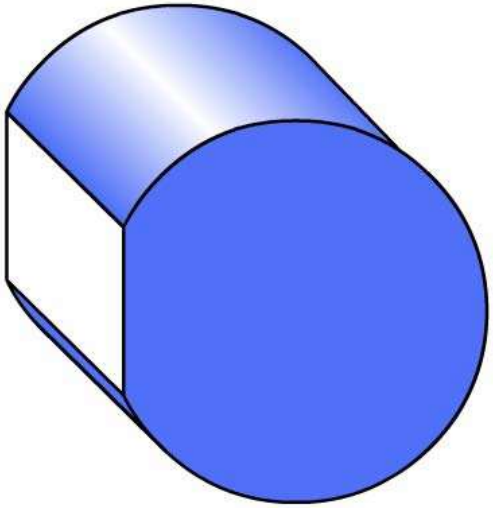


Cylindrical Grinding

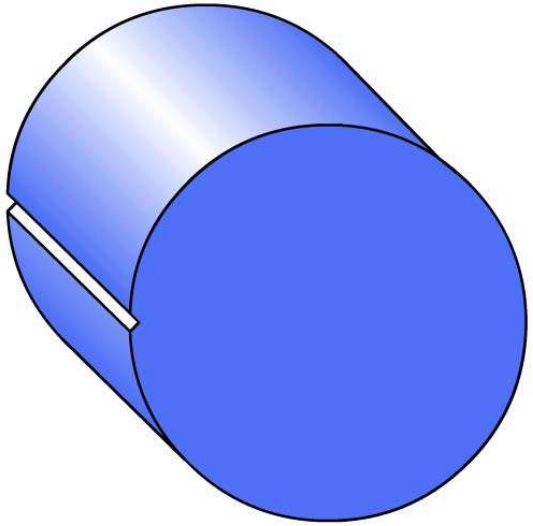


Thereafter, the single crystal gets marked by a “flat” or a notch

Flat, 150mm and smaller



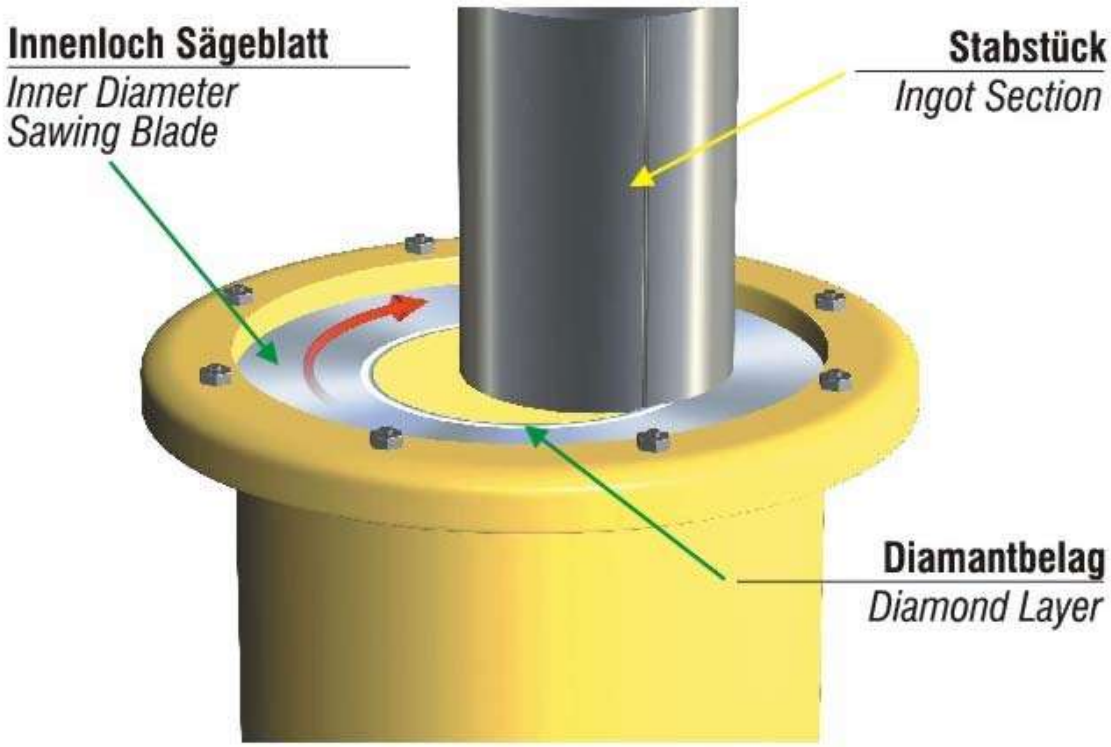
Notch, 200mm and larger



2.3 From crystal to wafer – inside hole saw -

The single crystal ingots are now cut into sections as a preparation for the subsequent wire saws. This happens with an inside hole saw (annular saw).

Scheme of an inside hole saw



2.3 From crystal to wafer - wire saw -

The wire saw is the most modern sawing method, and is standard for >= 300 mm wafer diameters.

Scheme of a wire saw

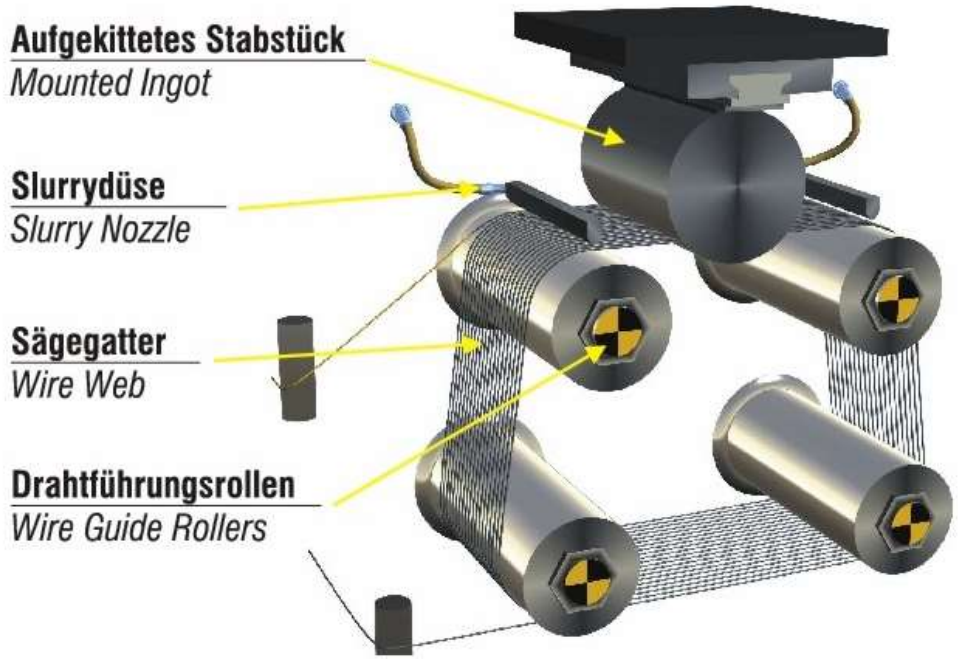
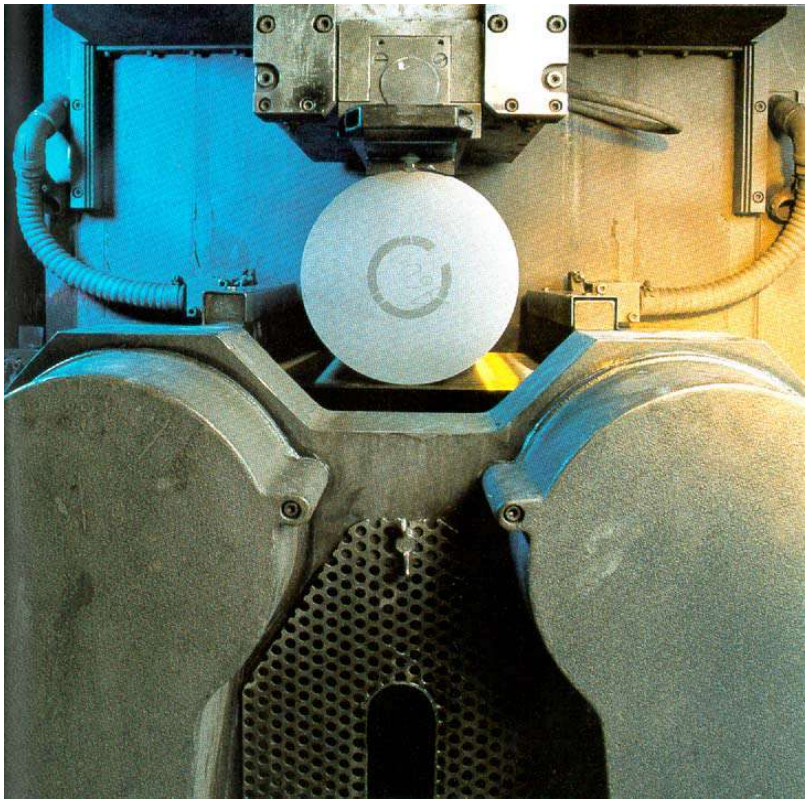
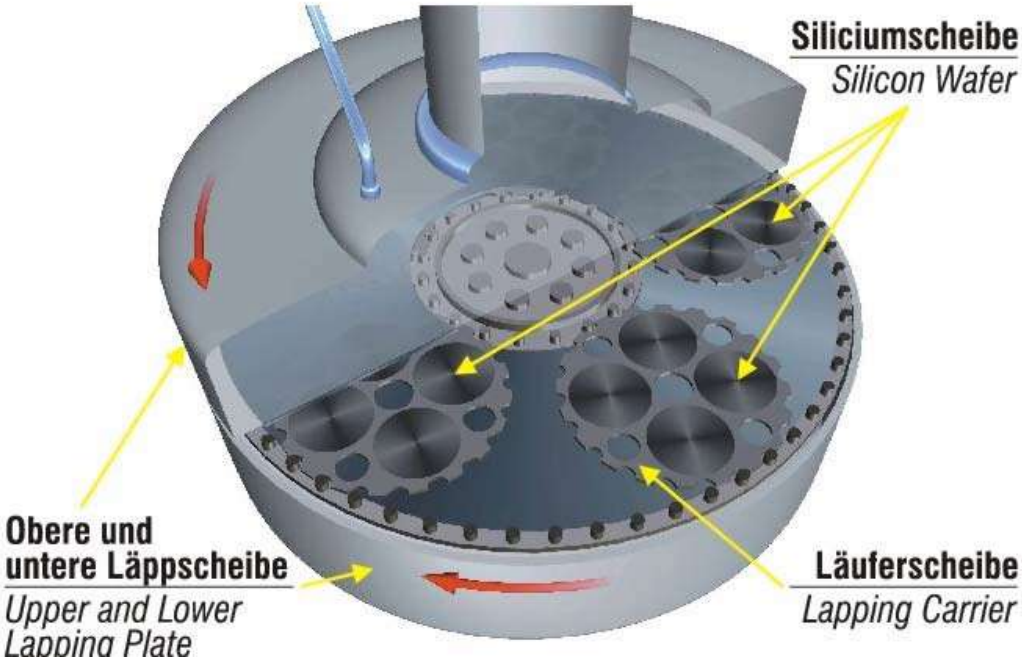


Photo of a wire saw

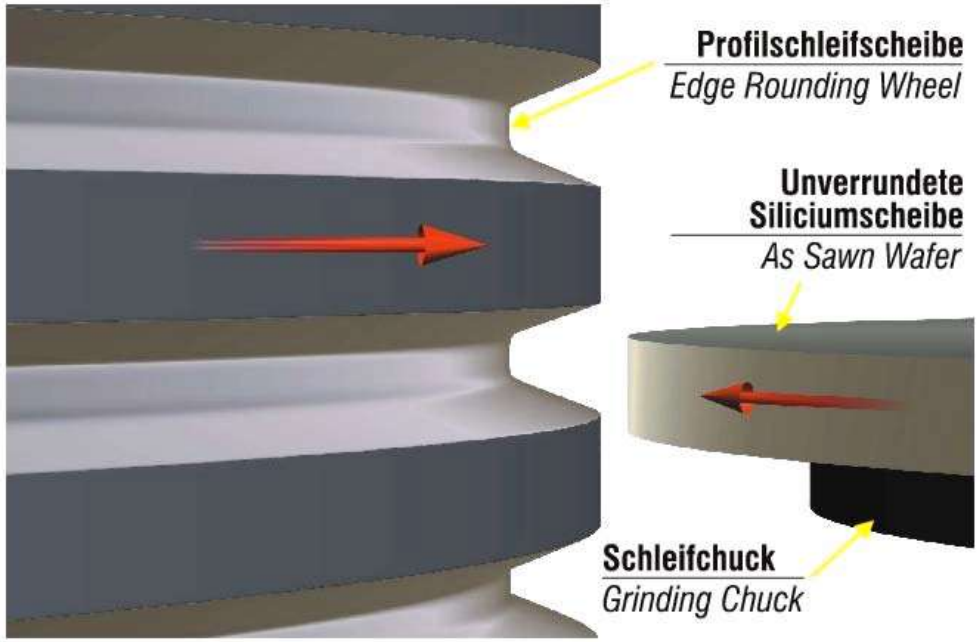


The wafers are now *lapped* and their edges will *rounded* to decrease the risk of fracture

Scheme of a tool for lapping

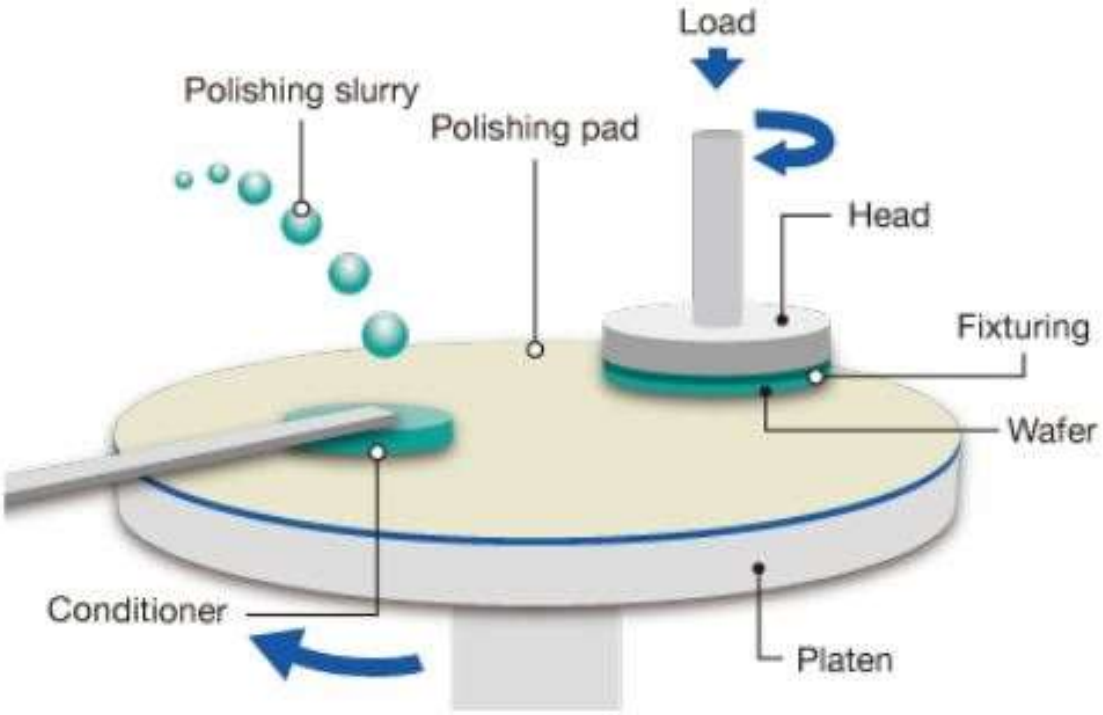


Edge rounding of the wafers



Now, the wafers are etched and polished using chemomechanical polishing (CMP). In Chapter 6 this method will be further discussed.

Schematic of a CMP tool



Finally, the wafers are polished one more time.

Scheme of a polishing plant

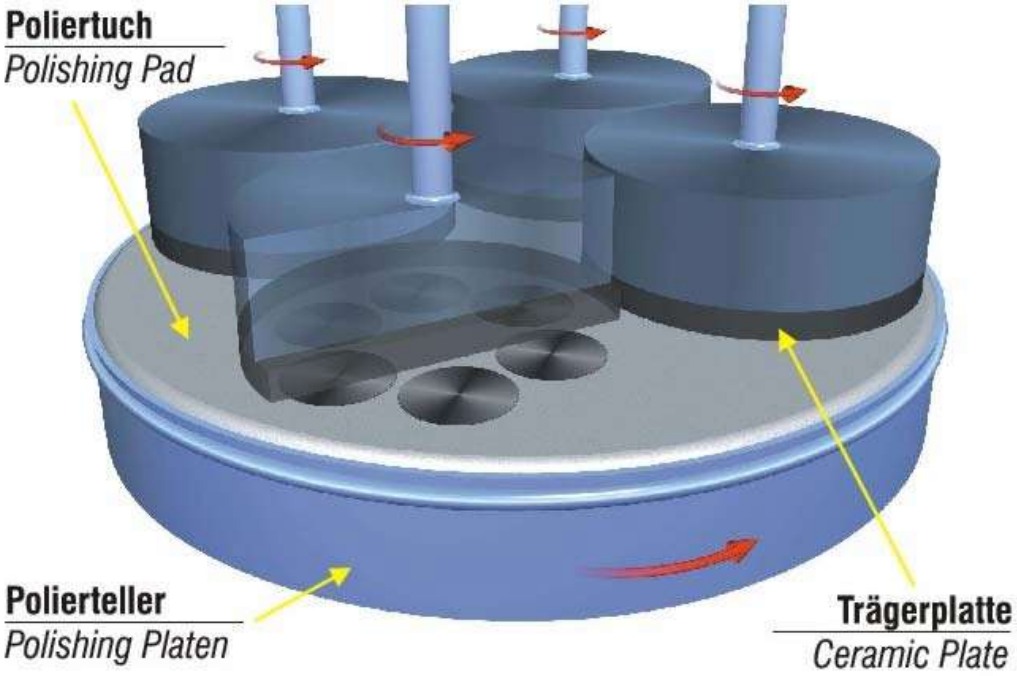
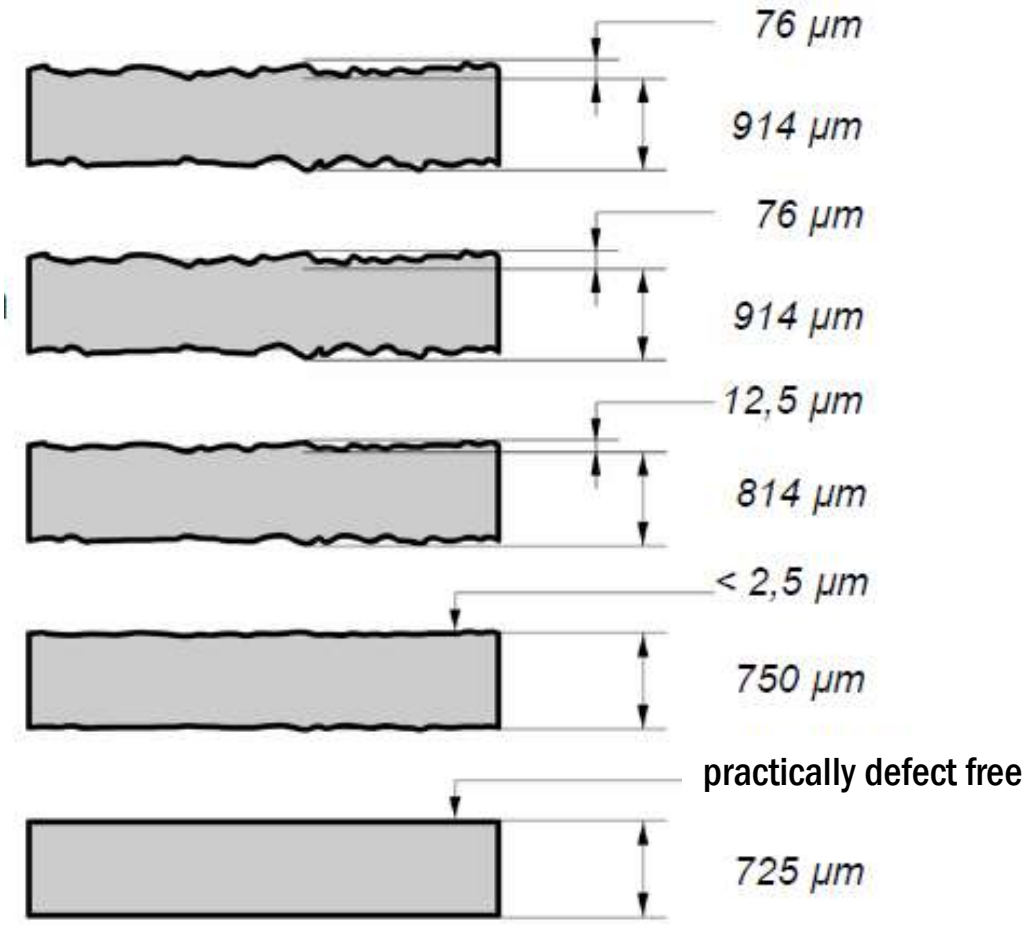


Photo of a polishing station

Change in slice thickness and surface roughness after different Process steps :

- after sawing
- after edge rounding
- after lapping
- after etching
- after CMP (polishing)



https://www.youtube.com/watch?v=TZxD2ePrphY

Selected parameters of silicon wafers :

Wafer diameter (mm)	Wafer thickness (μm)	Area (cm^2)	Weight (g)
50,8 (2 inch)	279	20,26	1,32
76,2 (3 inch)	381	45,61	4,05
100	525	78,65	9,67
125	625	112,72	17,87
150	675	176,72	27,82
200	725	314,16	52,98
300	775	706,21	127,62

Summary

✓Solids are divided into amorphous, crystalline, and crystalline, in turn, into poly- and monocrystalline

✓There are 14 different Bravais grids

✓Atomic positions, planes and families in crystal lattices are described with the Miller indices

✓Silicon crystallizes in the diamond lattice, which consists of two offset face-centered cubic lattices

✓Metallurgical silicon is cleaned using the Siemens or silane process and converted into polycrystalline Si

✓There are two methods for producing single crystals: Czochralski and float zone methods. Due to the absence of a crucible, the FZ process can produce purer silicon

✓The following production steps must be carried out to manufacture wafers: Cylindrical grinding, marking, sawing, lapping, edge rounding, CMP, polishing