# CRYSTALLOGRAPHY OF SILICON

# The Crystal Structure of Silicon

Silicon crystallises in the so-called diamond lattice in which each atom covalently binds tetrahedrally four adjacent atoms equivalently. The angle between the two binding partners of an atom is 109.5°, the distance between of the centres of two bonded atoms 2.35 Å (Fig. 6).

From these binding conditions of each Si atom, which can still be described in an illustrative manner, an astonishingly complex crystal structure results, which requires some spatial imagination. The following sections attempt to illustrate the spatial geometry of silicon crystals and their crystal axes and planes with the help of appropriate graphics.

## The Design of Silicon's Diamond Lattice

In order to construct a diamond lattice in an orthogonal coordinate system in which all three main axes are perpendicular to one another, a cubic surface-centred lattice is started as shown in Fig. 7, in which the atoms occupy all the corners and centres of sides of a diced elementary cell of the edge length 5.43 Å. The red reference lines do not correspond to the bonding ratios of the atoms, but to the edges of the elementary cells.

A copy of this lattice (Fig. 7, green reference lines as edges of the elementary cells) is now "integrated" into the first lattice in all three spatial directions displaced by a quarter of this edge length.

By connecting each atom with its four nearest neighbours (Fig. 7, yellow lines as Si-Si bonds) and hiding the edges of the elementary cells, one finally obtains the structure of the diamond lattice of silicon in which each silicon atom tetrahedrally binds four further silicon atoms as shown in Fig. 6.

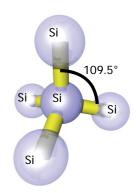


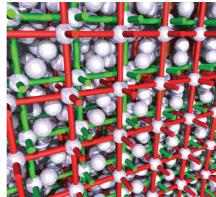
Fig. 6: Four more Si atoms bond to each Si atom In the silicon crystal.

# The Nomenclature of the Crystal Axes, Directions and Levels in the Diamond Lattice

The main crystal axis <100> is representative of the six direction vectors [100], [1'00], [010], [01'0], [001] and [001'] from the origin of the cubic elementary cell parallel to its edges. The main crystallographic plane {100} comprises the faces (100), (1'00), (010), (01'0), (001) and (001') perpendicular to these vectors which correspond to the side faces of the elementary cell.

The main crystal axis <110> denotes the twelve direction vectors [110], [101], [011], [1'10], [1'01], [01'1], [11'0], [101'], [101'], [101'], [1'10], [1'01'] and [01'1'] from the origin of the elementary cell along its side surface diagonals. To this end, the main crystallographic plane  $\{110\}$  with the surface array (110), (101)





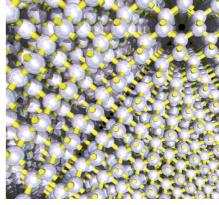


Fig. 7: A face-centred cubic lattice (left, unit cells marked with red edges), the same but additionally shifted in all directions by a quarter unit cell (centre, unit cells marked with green edges) results in the diamond lattice of silicon (right, unit cells without marking). The yellow bars correspond to the tetrahedral Si-Si bonds in the silicon lattice.

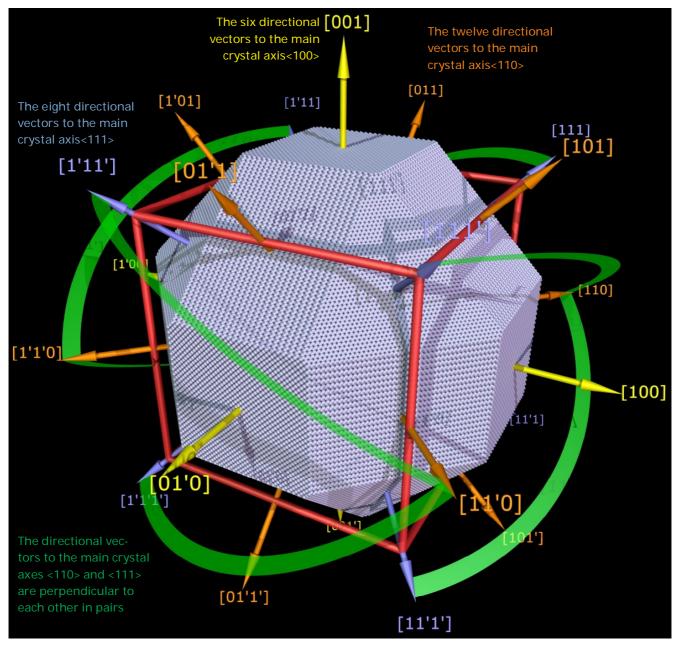
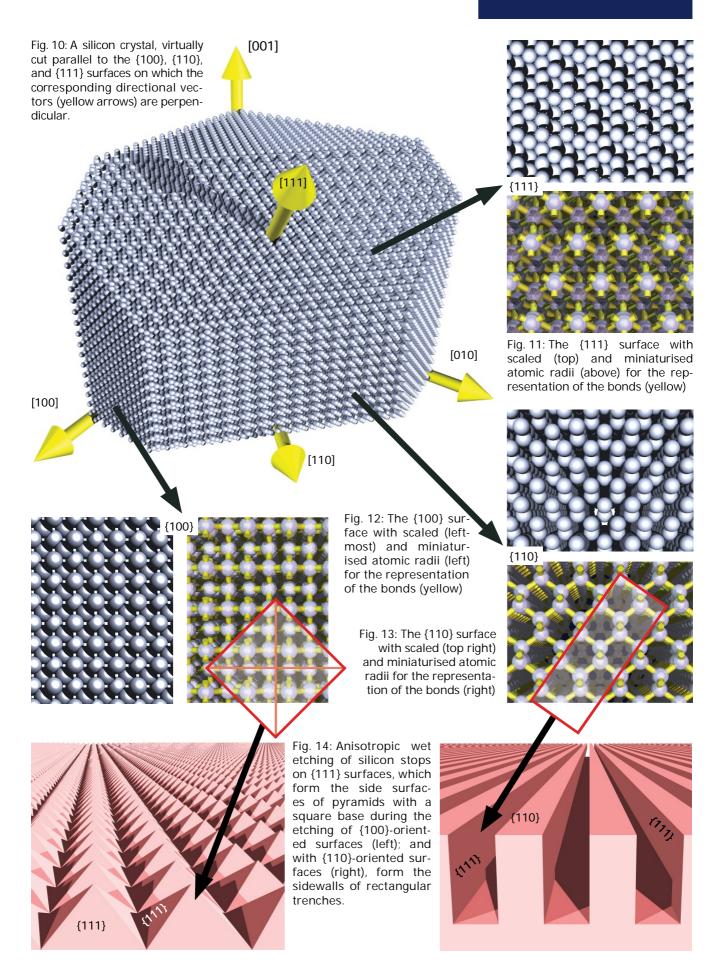


Fig. 8: A schematic silicon crystal with the 26 directional vectors along the three main crystal directions, with the position and orientation of the unit cell as a red wire model (greatly enlarged, not drawn to scale with respect to the Si atoms). Six directional vectors lie parallel to the edges of the unit cell, corresponding to the main crystal direction <100>, twelve directional vectors (corresponding to the main crystal direction <110>), parallel to the face diagonals of the unit cell, and eight directional vectors along the space diagonals of the unit cell (corresponding to the main crystal direction <111>).

The main crystal axis <111> comprises the eight direction vectors [111], [1'11], [11'1], [11'1], [1'11'], [1'11'], [1'11'] and [1'1'1'] from the origin of the elementary cell along its space diagonals. To this end, the main crystallographic plane {111} with the surface array (111), (1'11), (1'11), (11'1), (1'11'), (1'11') and (1'11') is located perpendicularly.

# MicroChemicals



## **Our Photoresists: Application Areas and Compatibilities**

	Recommended Applications 1	Resist Family	Photoresists	Resist Film Thickness <sup>2</sup>	Recommended Developers <sup>3</sup>	Recommended Removers 4	
Positive	Improved adhesion for wet etching, no focus on steep resist sidewalls	AZ <sup>®</sup> 1500	AZ <sup>®</sup> 1505 AZ <sup>®</sup> 1512 HS AZ <sup>®</sup> 1514 H AZ <sup>®</sup> 1518	≈ 0.5 µm ≈ 1.0 - 1.5 µm ≈ 1.2 - 2.0 µm ≈ 1.5 - 2.5 µm	AZ <sup>®</sup> 351B, AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF, AZ <sup>®</sup> Developer	AZ <sup>®</sup> 100 Remover, — TechniStrip <sup>®</sup> P1316 — TechniStrip <sup>®</sup> P1331	
		AZ <sup>®</sup> 4500	AZ <sup>®</sup> 4533 AZ <sup>®</sup> 4562	≈ 3 - 5 µm ≈ 5 - 10 µm	AZ <sup>®</sup> 400K, AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF, AZ <sup>®</sup> 826 MIF		
		AZ <sup>®</sup> P4000	AZ <sup>®</sup> P4110 AZ <sup>®</sup> P4330 AZ <sup>®</sup> P4620 AZ <sup>®</sup> P4903	≈ 1 - 2 µm ≈ 3 - 5 µm ≈ 6 - 20 µm ≈ 10 - 30 µm	AZ <sup>®</sup> 400K, AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF, AZ <sup>®</sup> 826 MIF		
		AZ <sup>®</sup> PL 177 AZ <sup>®</sup> 4999	AZ <sup>®</sup> PL 177		AZ® 351B, AZ® 400K, AZ® 326 MIF, AZ® 726 MIF, AZ® 826 MIF		
	Spray coating  Dip coating	MC Dip Coating Resist			AZ® 400K, AZ® 326 MIF, AZ® 726 MIF, AZ® 826 MIF AZ® 351B, AZ® 400K, AZ® 326 MIF, AZ® 726 MIF, AZ® 826 MIF		
	Steep resist sidewalls, high resolution and aspect ratio for e. g. dry etching or plating	AZ® ECI 3000	AZ <sup>®</sup> ECI 3007 AZ <sup>®</sup> ECI 3012 AZ <sup>®</sup> ECI 3027	≈ 0.7 µm ≈ 1.0 - 1.5 µm ≈ 2 - 4 µm	AZ <sup>®</sup> 351B, AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF, AZ <sup>®</sup> Developer		
		AZ® 9200	AZ <sup>®</sup> 9245 AZ <sup>®</sup> 9260	≈ 3 - 6 µm ≈ 5 - 20 µm			
	Elevated thermal softening point and high resolution for e. g. dry etching	AZ® 701 MiR	AZ <sup>®</sup> 701 MiR (14 cPs) AZ <sup>®</sup> 701 MiR (29 cPs)	≈ 0.8 µm ≈ 2 - 3 µm	AZ <sup>®</sup> 351B, AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF, AZ <sup>®</sup> Developer		
Positive (chem. amplified)	Steep resist sidewalls, high resolution and aspect ratio for e. g. dry etching or plating	AZ <sup>®</sup> XT AZ <sup>®</sup> IPS 6050	AZ <sup>®</sup> 12 XT-20PL-05 AZ <sup>®</sup> 12 XT-20PL-10 AZ <sup>®</sup> 12 XT-20PL-20 AZ <sup>®</sup> 40 XT	≈ 15 - 50 µm	AZ <sup>®</sup> 400K, AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF	AZ <sup>®</sup> 100 Remover, TechniStrip <sup>®</sup> P1316 TechniStrip <sup>®</sup> P1331	
			LA7® 5000	≈ 20 - 100 µm			
Image Re- versal	Elevated thermal softening point and undercut for lift-off applications	AZ <sup>®</sup> 5200	AZ <sup>®</sup> 5209 AZ <sup>®</sup> 5214 TI 35ESX	≈ 1 µm ≈ 1 - 2 µm ≈ 3 - 4 µm	AZ <sup>®</sup> 351B, AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF	TechniStrip <sup>®</sup> Micro D2 TechniStrip <sup>®</sup> P1316 TechniStrip <sup>®</sup> P1331	
<del>ار</del> 8		TI	TI xLift-X	≈ 4 - 8 µm			
Negative (Cross-linking)	Negative resist sidewalls in combination with no thermal softening for lift-off application	AZ <sup>®</sup> nLOF 2000	AZ <sup>®</sup> nLOF 2020 AZ <sup>®</sup> nLOF 2035 AZ <sup>®</sup> nLOF 2070	≈ 1.5 - 3 µm ≈ 3 - 5 µm ≈ 6 - 15 µm	AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF, AZ <sup>®</sup> 826 MIF	TechniStrip® NI555 TechniStrip® NF52 TechniStrip® MLO 07	
		AZ <sup>®</sup> nLOF 5500	AZ <sup>®</sup> nLOF 5510	≈ 0.7 - 1.5 µm			
	Improved adhesion, steep resist sidewalls and high aspect ratios for e. g. dry etching or plating		AZ <sup>®</sup> 15 nXT (115 cPs) AZ <sup>®</sup> 15 nXT (450 cPs)	≈ 2 - 3 µm ≈ 5 - 20 µm	AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF, AZ <sup>®</sup> 826 MIF	Technistrip* MLO 07	
		AZ <sup>®</sup> nXT	AZ <sup>®</sup> 125 nXT	≈ 20 - 100 µm	AZ <sup>®</sup> 326 MIF, AZ <sup>®</sup> 726 MIF, AZ <sup>®</sup> 826 MIF	TechniStrip® P1316 TechniStrip® P1331 TechniStrip® NF52 TechniStrip® MLO 07	

# **Our Developers: Application Areas and Compatibilities**

#### **Inorganic Developers**

(typical demand under standard conditions approx. 20 L developer per L photoresist)

AZ® Developer is based on sodium phosphate and –metasilicate, is optimized for minimal aluminum attack and is typically used diluted 1:1 in DI water for high contrast or undiluted for high development rates. The dark erosion of this developer is slightly higher compared to other developers.

AZ® 351B is based on buffered NaOH and typically used diluted 1:4 with water, for thick resists up to 1:3 if a lower contrast can be tolerated.

AZ® 400K is based on buffered KOH and typically used diluted 1 : 4 with water, for thick resists up to 1 : 3 if a lower contrast can be tolerated.

AZ® 303 specifically for the AZ® 111 XFS photoresist based on KOH / NaOH is typically diluted 1:3-1:7 with water, depending on whether a high development rate, or a high contrast is required

# Metal Ion Free (TMAH-based) Developers

(typical demand under standard conditions approx. 5 - 10 L developer concentrate per L photoresist)

AZ® 326 MIF is 2.38 % TMAH- (TetraMethylAmmoniumHydroxide) in water.

<sup>2</sup> Resist film thickness achievable and processable with standard equipment under standard conditions. Some resists can be diluted for lower film thicknesses, with additional effort also thicker resist films can be achieved and processed. reasonable if metal ion free development is reAZ® 726 MIF is 2.38 % TMAH- (TetraMethylAmmoniumHydroxide) in water, with additional surfactants for rapid and uniform wetting of the substrate (e. g. for puddle development)

**AZ® 826 MIF** is 2.38 % TMAH- (<u>TetraMethylAmmoniumHy</u>droxide) in water, with additional surfactants for rapid and uniform wetting of the substrate (e. g. for puddle development) and other additives for the removal of poorly soluble resist components (residues with specific resist families), however at the expense of a slightly higher dark erosion.

## Our Removers: Application Areas and Compatibilities

AZ<sup>®</sup> 100 Remover is an amine solvent mixture and standard remover for AZ<sup>®</sup> and TI photoresists. To improve its performance, AZ<sup>®</sup> 100 remover can be heated to 60 - 80°C. Because the AZ<sup>®</sup> 100 Remover reacts highly alkaline with water, it is suitable for this with respect to sensitive substrate materials such as Cu, Al or ITO only if contamination with water can be ruled out..

**TechniStrip® P1316** is a remover with very strong stripping power for Novolak-based resists (including all AZ® positive resists), epoxy-based coatings, polyimides and dry films. At typical application temperatures around 75°C, TechniStrip® P1316 may dissolve cross-linked resists without residue also, e.g. through dry etching or ion implantation. TechniStrip® P1316 can also be used in spraying processes. For alkaline sensitive materials, TechniStrip® P1331 would be an alternative to the P1316. Nicht kompatibel mit Au oder GaAs.

TechniStrip® P1331 can be an alternative for TechniStrip® P1316 in case of alkaline sensitive materials. TechniStrip® P1331 is not compatible with Au or GaAs.

**TechniStrip**® **NI555** is a stripper with very strong dissolving power for Novolak-based negative resists such as the AZ® 15 nXT and AZ® nLOF 2000 series and very thick positive resists such as the AZ® 40 XT. TechniStrip® NI555 was developed not only to peel cross-linked resists, but also to dissolve them without residues. This prevents contamination of the basin and filter by resist particles and skins, as can occur with standard strippers. TechniStrip® NI555 is not compatible with GaAs.

TechniClean<sup>TM</sup> CA25 is a semi-aqueous proprietary blend formulated to address post etch residue (PER) removal for all interconnect and technology nodes. Extremely efficient at quickly and selectively removing organo-metal oxides from Al. Cu. Ti. TiN. W and Ni.

TechniStrip™ NF52 is a highly effective remover for negative resists (liquid resists as well as dry films). The intrinsic nature of the additives and solvent make the blend totally compatible with metals used throughout the BEOL interconnects to WLP bumping applications.

**TechniStrip™ Micro D2** is a versatile stripper dedicated to address resin lift-off and dissolution on negative and positive tone resist. The organic mixture blend has the particularity to offer high metal and material compatibility allowing to be used on all stacks and particularly on fragile III/V substrates for instance.

**TechniStrip™ MLO 07** is a highly efficient positive and negative tone photoresist remover used for IR, III/V, MEMS, Photonic, TSV mask, solder bumping and hard disk stripping applications. Developed to address high dissolution performance and high material compatibility on Cu, Al, Sn/Ag, Alumina and common organic substrates.

## Our Wafers and their Specifications

#### Silicon-, Quartz-, Fused Silica and Glass Wafers

Silicon wafers are either produced via the Czochralski- (CZ-) or Float zone- (FZ-) method. The more expensive FZ wafers are primarily reasonable if very high-ohmic wafers (> 100 Ohm cm) are required.

Quartz wafers are made of monocrystalline SiO<sub>2</sub>, main criterion is the crystal orientation (e. g. X-, Y-, Z-, AT- or ST-cut)

Fused silica wafers consist of amorphous SiO₂. The so-called JGS2 wafers have a high transmission in the range of ≈ 280 - 2000 nm wavelength, the more expensive JGS1 wafers at ≈ 220 - 1100 nm.

Our glass wafers, if not otherwise specified, are made of borosilicate glass.

### **Specifications**

Common parameters for all wafers are diameter, thickness and surface (1- or 2-side polished). Fused silica wafers are made either of JGS1 or JGS2 material, for quartz wafers the crystal orientation needs to be defined. For silicon wafers, beside the crystal orientation (<100> or <111>) the doping (n- or p-type) as well as the resistivity (Ohm cm) are selection criteria.

#### Prime-, Test-, and Dummy Wafers

Silicon wafers usually come as "Prime-grade" or "Test-grade", latter mainly have a slightly broader particle specification. "Dummy-Wafers" neither fulfill Prime- nor Test-grade for different possible reasons (e. g. very broad or missing specification of one or several parameters, reclaim wafers, no particle specification) but might be a cheap alternative for e. g. resist coating tests or equipment start-up.

#### Our Silicon-, Quartz-, Fused Silica and Glass Wafers

Our frequently updated wafer stock list can be found here:

è www.microchemicals.com/products/wafers/waferlist.html

#### **Further Products from our Portfolio**

#### **Plating**

Plating solutions for e. g. gold, copper, nickel, tin or palladium:

è www.microchemicals.com/products/electroplating.html

Solvents (MOS, VLSI, ULSI)

Acetone, isopropyl alcohol, MEK, DMSO, cyclopentanone, butylacetate, ... è www.microchemicals.com/products/solvents.html

Acids and Bases (MOS, VLSI, ULSI)

Hydrochloric acid, sulphuric acid, nitric acid, KOH, TMAH, ... è www.microchemicals.com/products/etchants.html

**Etching Mixtures** 

for e. g. chromium, gold, silicon, copper, titanium, ...

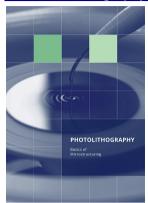
è www.microchemicals.com/products/etching mixtures.html

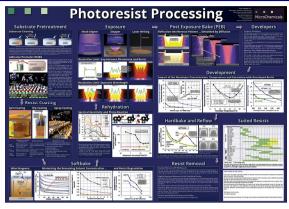
## **Further Information**

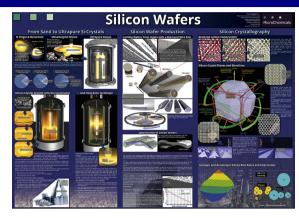
Technical Data Sheets: www.microchemicals.com/downloads/product\_data\_sheets/photoresists.html

Material Safety Data Sheets (MSDS): www.microchemicals.com/downloads/safety\_data\_sheets/msds\_links.html

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