# 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.

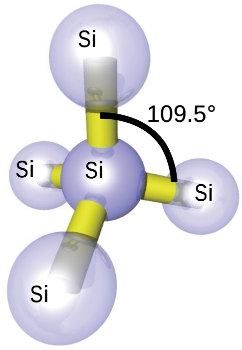



Fig. 6: Four more Si atoms bond to each Si atom In the silicon crystal.

## 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.

## 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'], [011'], [1'1'0], [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), (011), (1'10), (1'01), (01'1) ), (011'), (1'1'0), (1'01') and (01'1') is located perpendicularly.

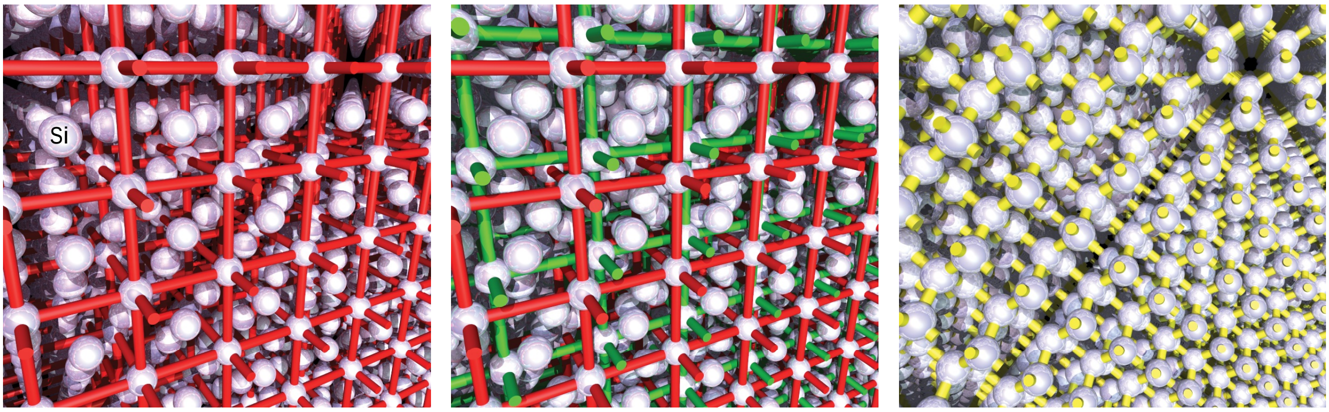



Fig. 7: A face-centred cubic lattice (left, unit cells marked with red edges), the same but additionally shifted in all directions by a quarter unit cell (centre, unit cells marked with green edges) results in the diamond lattice of silicon (right, unit cells without marking). The yellow bars correspond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

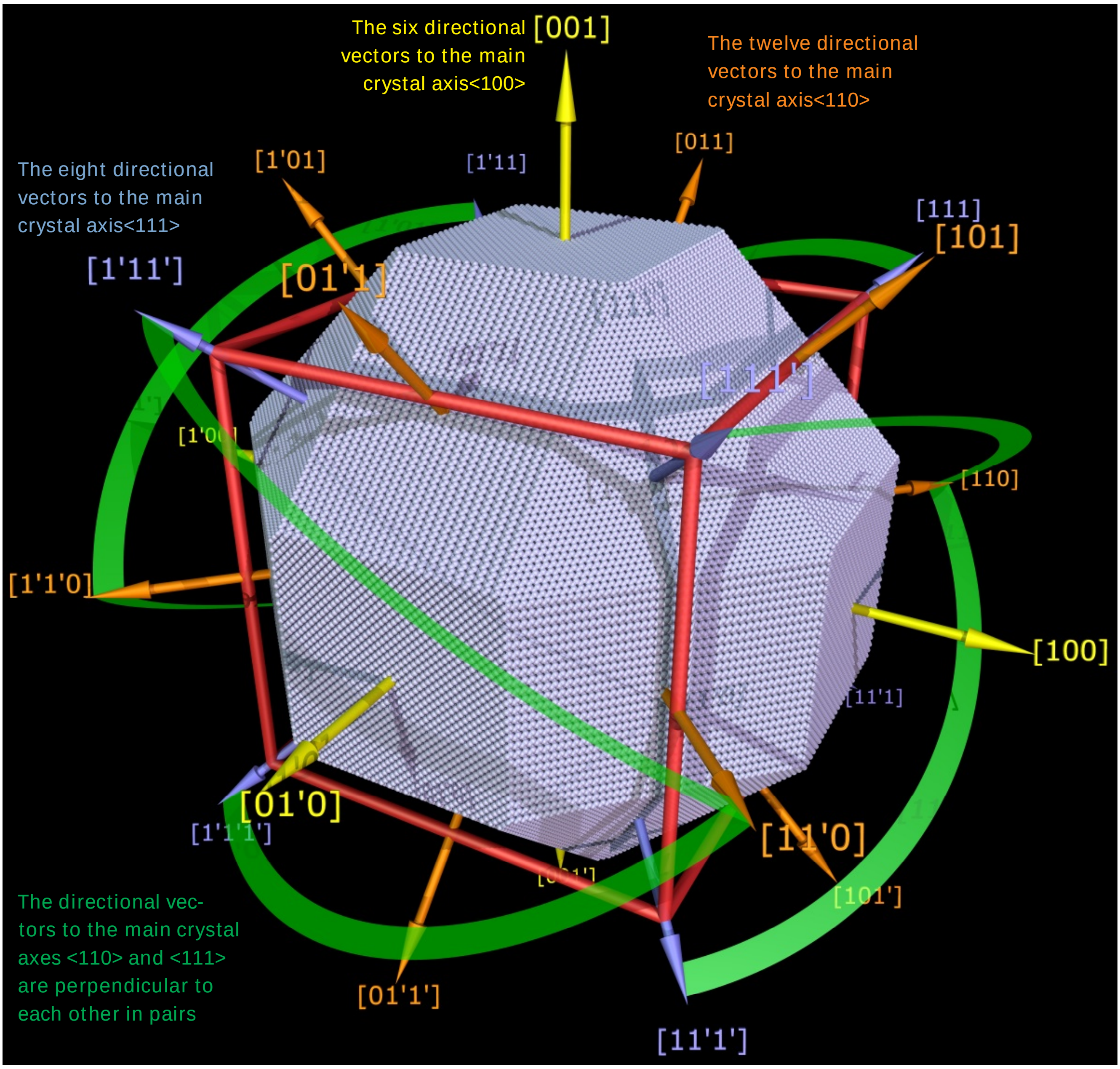



Fig. 8: A schematic silicon crystal with the 26 directional vectors along the three main crystal directions, with the position and orientation of the unit cell as a red wire model (greatly enlarged, not drawn to scale with respect to the Si atoms). Six directional vectors lie parallel to the edges of 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], [111'], [1'1'1], [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), (11‘1), (111‘), (1‘1‘1), (1‘11‘), (1‘11‘) and (1‘1‘1‘) is located perpendicularly.

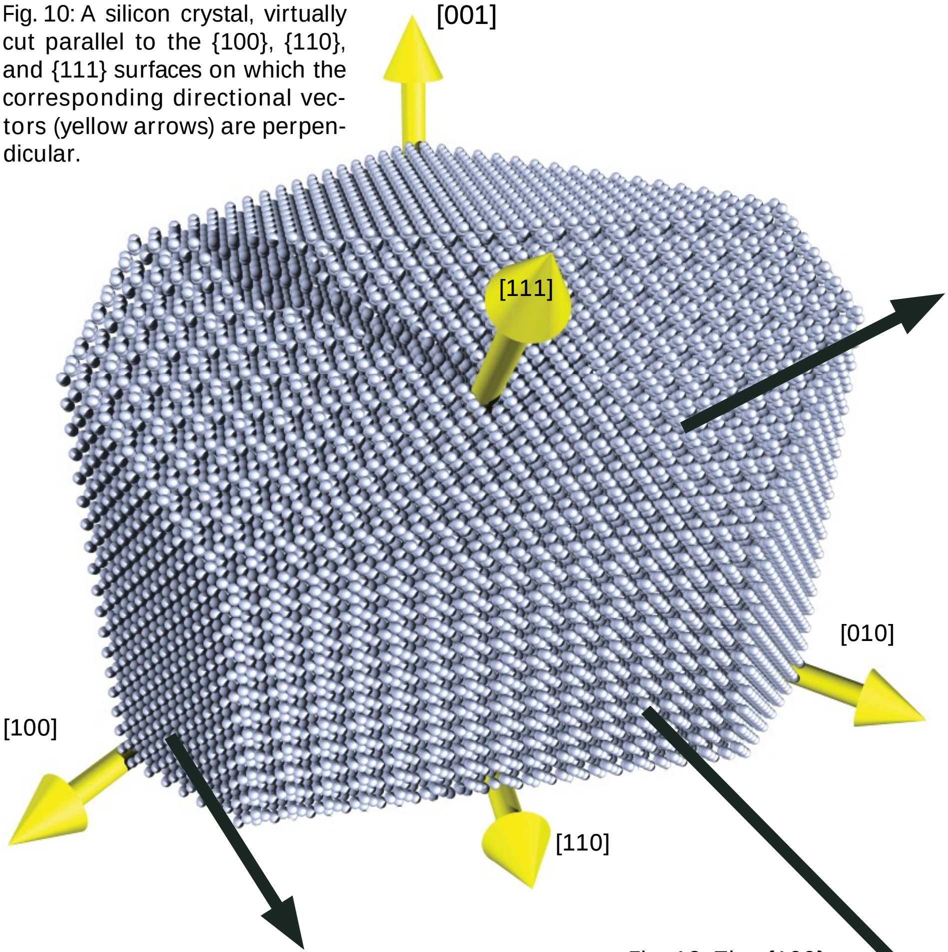



Fig. 10: A silicon crystal, virtually cut parallel to the {100}, {110}, and {111} surfaces on which the corresponding directional vectors (yellow arrows) are perpendicular.

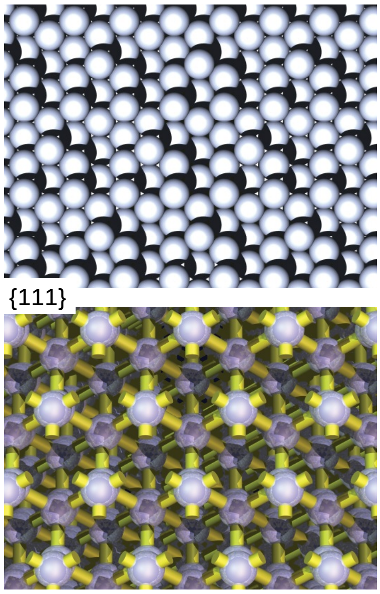



Fig. 11: The {111} surface with scaled (top) and miniaturised atomic radii (above) for the representation of the bonds (yellow)

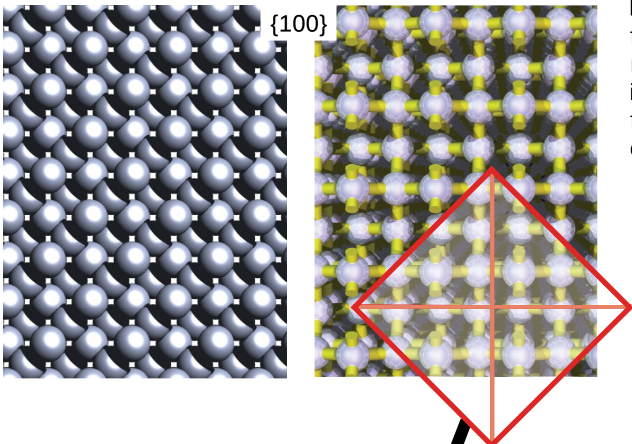



Fig. 12: The {100} surface with scaled (leftmost) and miniaturised atomic radii (left) for the representation of the bonds (yellow)

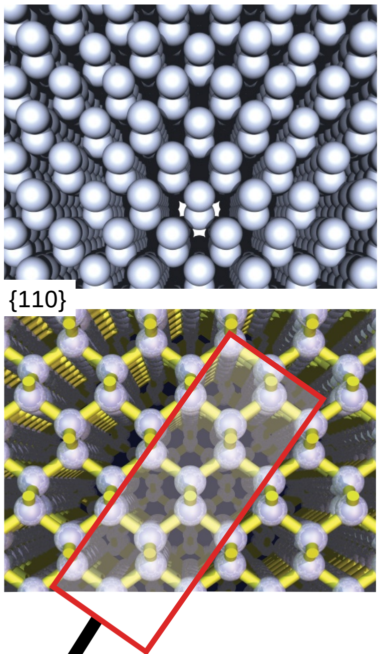
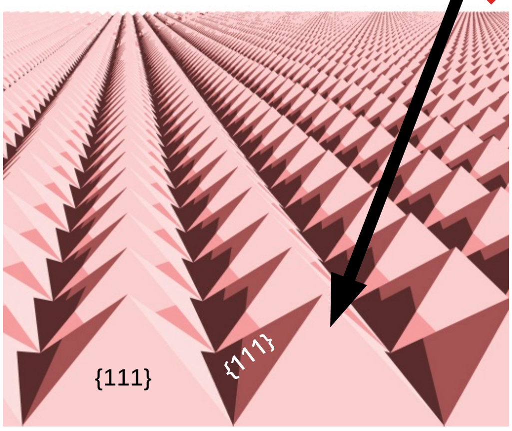



Fig. 13: The {110} surface with scaled (top right) and miniaturised atomic radii for the representation of the bonds (right)



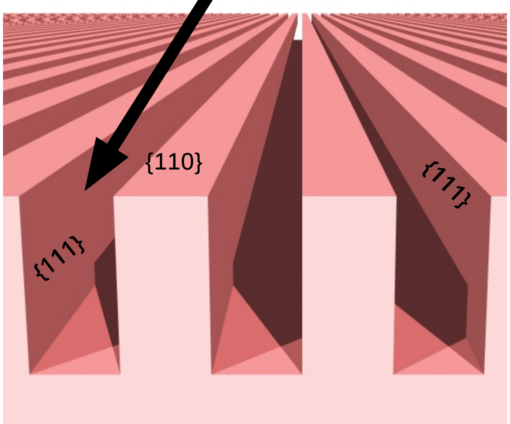




Fig. 14: Anisotropic wet etching of silicon stops on {111} surfaces, which form the side surfaces of pyramids with a square base during the etching of {100}-oriented surfaces (left); and with {110}-oriented surfaces (right), form the sidewalls of rectangular trenches.

## Our Photoresists: Application Areas and Compatibilities

| | Recommended Applications [1] | Resist Family | Photoresists | Resist Film Thickness [2] | Recommended Developers [3] | Recommended Re-movers [4] |
|---|---|---|---|---|---|---|
| Positive | Improved adhesion for wet etching, no focus on steep resist sidewalls | AZ® 1500 | AZ® 1505<br>AZ® 1512 HS<br>AZ® 1514 H<br>AZ® 1518 | ≈ 0.5 µm<br>≈ 1.0 - 1.5 µm<br>≈ 1.2 - 2.0 µm<br>≈ 1.5 - 2.5 µm | AZ® 351B, AZ® 326 MIF, AZ® 726 MIF, AZ® Developer | AZ® 100 Remover,<br>TechniStrip® P1316<br>TechniStrip® P1331 |
| | | AZ® 4500 | AZ® 4533<br>AZ® 4562 | ≈ 3 - 5 µm<br>≈ 5 - 10 µm | AZ® 400K, AZ® 326 MIF, AZ® 726 MIF, AZ® 2026 MIF | |
| | | AZ® P4000 | AZ® P4110<br>AZ® P4330<br>AZ® P4620<br>AZ® P4903 | ≈ 1 - 2 µm<br>≈ 3 - 5 µm<br>≈ 6 - 20 µm<br>≈ 10 - 30 µm | AZ® 400K, AZ® 326 MIF, AZ® 726 MIF, AZ® 2026 MIF | |
| | | AZ® PL 177 | AZ® PL 177 | ≈ 3 - 8 µm | AZ® 351B, AZ® 400K, AZ® 326 MIF, AZ® 726 MIF, AZ® 2026 MIF | |
| | Spray coating | AZ® 4999 | | ≈ 1 - 15 µm | AZ® 400K, AZ® 326 MIF, AZ® 726 MIF, AZ® 2026 MIF | |
| | Dip coating | MC Dip Coating Resist | | ≈ 2 - 15 µm | AZ® 351B, AZ® 400K, AZ® 326 MIF, AZ® 726 MIF, AZ® 2026 MIF | |
| | Steep resist sidewalls, high resolution and aspect ratio for e. g. dry etching or plating | AZ® ECI 3000 | AZ® ECI 3007<br>AZ® ECI 3012<br>AZ® ECI 3027 | ≈ 0.7 µm<br>≈ 1.0 - 1.5 µm<br>≈ 2 - 4 µm | AZ® 351B, AZ® 326 MIF, AZ® 726 MIF, AZ® Developer | |
| | | AZ® 9200 | AZ® 9245<br>AZ® 9260 | ≈ 3 - 6 µm<br>≈ 5 - 20 µm | AZ® 400K, AZ® 326 MIF, AZ® 726 MIF | |
| | Elevated thermal softening point and high resolution for e. g. dry etching | AZ® 701 MiR | AZ® 701 MiR (14 cPs)<br>AZ® 701 MiR (29 cPs) | ≈ 0.8 µm<br>≈ 2 - 3 µm | AZ® 351B, AZ® 326 MIF, AZ® 726 MIF, AZ® Developer | |
| Positive (chem. amplified) | Steep resist sidewalls, high resolution and aspect ratio for e. g. dry etching or plating | AZ® XT | AZ® 12 XT-20PL-05<br>AZ® 12 XT-20PL-10<br>AZ® 12 XT-20PL-20<br>AZ® 40 XT | ≈ 3 - 5 µm<br>≈ 6 - 10 µm<br>≈ 10 - 30 µm<br>≈ 15 - 50 µm | AZ® 400K, AZ® 326 MIF, AZ® 726 MIF | AZ® 100 Remover,<br>TechniStrip® P1316<br>TechniStrip® P1331 |
| | | AZ® IPS 6050 | | ≈ 20 - 100 µm | | |
| Image Re-versal | Elevated thermal softening point and undercut for lift-off applications | AZ® 5200 | AZ® 5209<br>AZ® 5214 | ≈ 1 µm<br>≈ 1 - 2 µm | AZ® 351B, AZ® 326 MIF, AZ® 726 MIF | TechniStrip® Micro D2<br>TechniStrip® P1316<br>TechniStrip® P1331 |
| | | TI | TI 35ESX<br>TI xLift-X | ≈ 3 - 4 µm<br>≈ 4 - 8 µm | | |
| Negative (Cross-linking) | Negative resist sidewalls in combination with no thermal softening for lift-off application | AZ® nLOF 2000 | AZ® nLOF 2020<br>AZ® nLOF 2035<br>AZ® nLOF 2070 | ≈ 1.5 - 3 µm<br>≈ 3 - 5 µm<br>≈ 6 - 15 µm | AZ® 326 MIF, AZ® 726 MIF, AZ® 2026 MIF | TechniStrip® NI555<br>TechniStrip® NF52<br>TechniStrip® MLO 07 |
| | | AZ® nLOF 5500 | AZ® nLOF 5510 | ≈ 0.7 - 1.5 µm | | |
| | Improved adhesion, steep resist side-walls and high aspect ratios for e. g. dry etching or plating | AZ® nXT | AZ® 15 nXT (115 cPs)<br>AZ® 15 nXT (450 cPs) | ≈ 2 - 3 µm<br>≈ 5 - 20 µm | AZ® 326 MIF, AZ® 726 MIF, AZ® 2026 MIF | |
| | | | AZ® 125 nXT | ≈ 20 - 100 µm | AZ® 326 MIF, AZ® 726 MIF, AZ® 2026 MIF | TechniStrip® P1316<br>TechniStrip® P1331<br>TechniStrip® NF52<br>TechniStrip® MLO 07 |

*[1] In general, almost all resists can be used for almost any application. However, the special properties of each resist family makes them specially suited for certain fields of application.*
*[2] 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.*
*[3] Metal ion free (MIF) developers are significantly more expensive, and reasonable if metal ion free development is required.*

## 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.

**AZ® 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- (TetraMethylAmmoniumHydroxide) 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® 100 Remover** is an amine solvent mixture and standard remover for AZ® and TI photoresists. To improve its performance, AZ® 100 remover can be heated to 60 - 80°C. Because the AZ® 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. Not compatible with Au.

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

**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™ 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 $SiO_2$, main criterion is the crystal orientation (e. g. X-, Y-, Z-, AT- or ST-cut)

Fused silica wafers consist of amorphous $SiO_2$. 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

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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

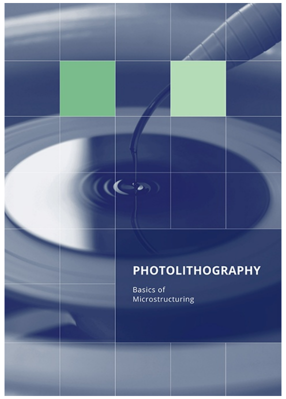
**Etching Mixtures**

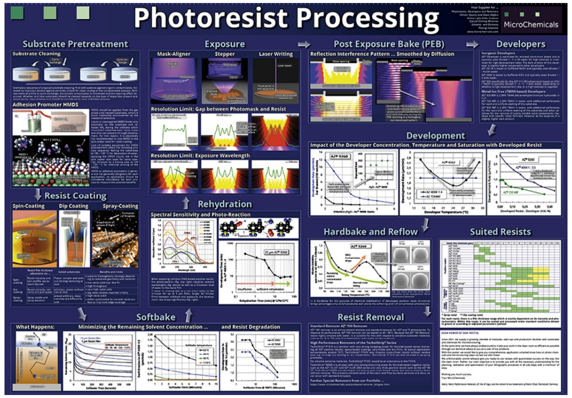
for e. g. chromium, gold, silicon, copper, titanium, ... **è** www.microchemicals.com/products/etching_mixtures.html

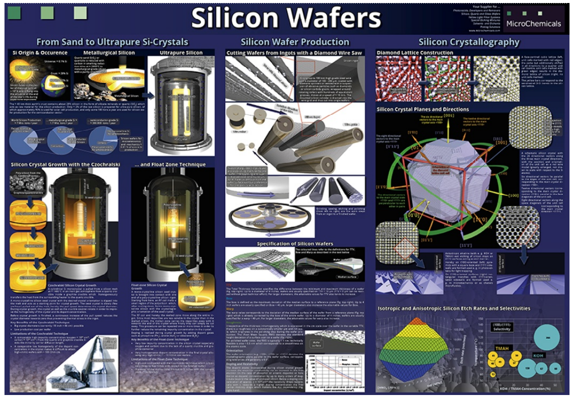
## Further Information

| | |
|---|---|
| **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 |

## Our Photolithography Book and -Posters

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