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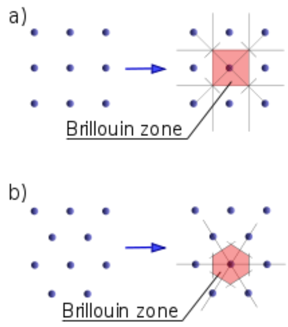
Brillouin zone

In mathematics and solid state physics, the first **Brillouin zone** is a uniquely defined primitive cell in reciprocal space. In the same way the Bravais lattice is divided up into Wigner–Seitz cells in the real lattice, the reciprocal lattice is broken up into Brillouin zones. The boundaries of this cell are given by planes related to points on the reciprocal lattice. The importance of the Brillouin zone stems from the Bloch wave description of waves in a periodic medium, in which it is found that the solutions can be completely characterized by their behavior in a single Brillouin zone.

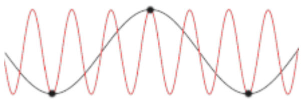


The reciprocal lattices (dots) and corresponding first Brillouin zones of (a) square lattice and (b) hexagonal lattice.

The first Brillouin zone is the locus of points in reciprocal space that are closer to the origin of the reciprocal lattice than they are to any other reciprocal lattice points (see the derivation of the Wigner–Seitz cell). Another definition is as the set of points in *k*-space that can be reached from the origin without crossing any Bragg plane. Equivalently, this is the Voronoi cell around the origin of the reciprocal lattice.

There are also second, third, *etc.*, Brillouin zones, corresponding to a sequence of disjoint regions (all with the same volume) at increasing distances from the origin, but these are used less frequently. As a result, the *first* Brillouin zone is often called simply the *Brillouin zone*. In general, the *n*-th Brillouin zone consists of the set of points that can be reached from the origin by crossing exactly $n-1$ distinct Bragg planes. A related concept is that of the **irreducible Brillouin zone**, which is the first Brillouin zone reduced by all of the symmetries in the point group of the lattice (point group of the crystal).

The concept of a Brillouin zone was developed by Léon Brillouin (1889–1969), a French physicist.

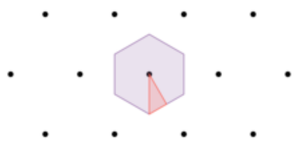

k-vectors exceeding the first Brillouin zone (red) do not carry any more information than their counterparts (black) in the first Brillouin zone. k at the Brillouin zone edge is the spatial Nyquist frequency of waves in the lattice, because it corresponds to a half-wavelength equal to the inter-atomic lattice spacing *a*.[1] See also Aliasing § Sampling sinusoidal functions for more on the equivalence of k-vectors.

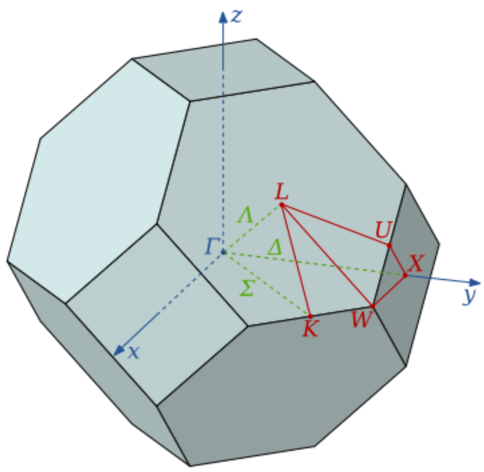
Contents

Critical points

Several points of high symmetry are of special interest – these are called critical points.[2]

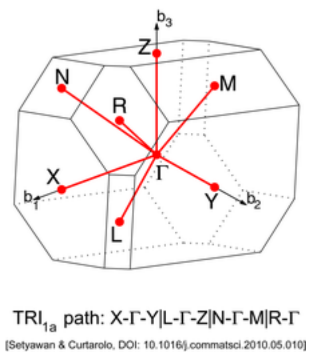
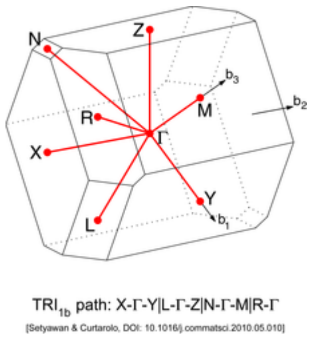
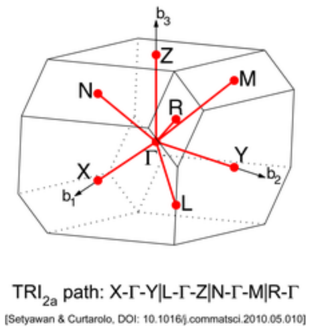
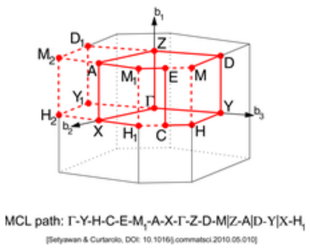
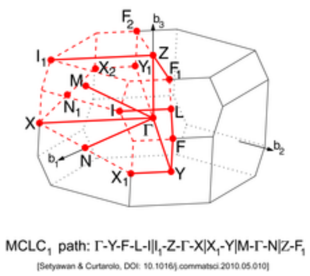
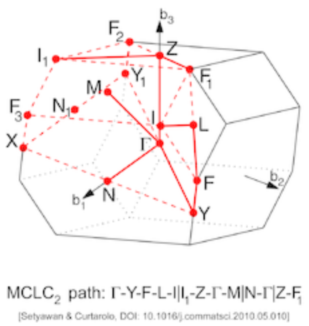
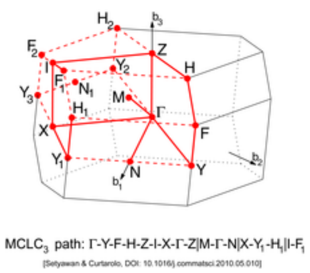
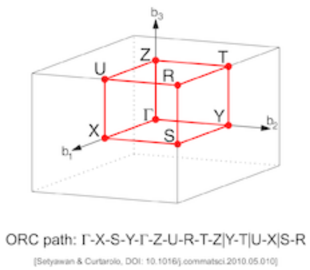
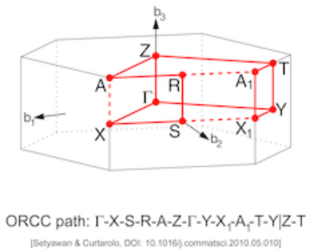
Symbol	Description
Γ	Center of the Brillouin zone
	Simple cube
M	Center of an edge
R	Corner point
X	Center of a face
	Face-centered cubic
K	Middle of an edge joining two hexagonal faces
L	Center of a hexagonal face
U	Middle of an edge joining a hexagonal and a square face
W	Corner point
X	Center of a square face
	Body-centered cubic
H	Corner point joining four edges
N	Center of a face
P	Corner point joining three edges
	Hexagonal
A	Center of a hexagonal face
H	Corner point
K	Middle of an edge joining two rectangular faces
L	Middle of an edge joining a hexagonal and a rectangular face
M	Center of a rectangular face

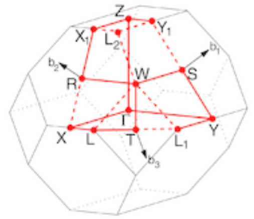
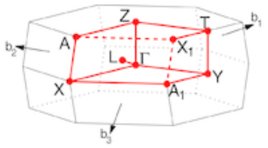
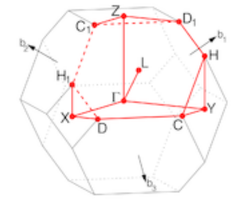
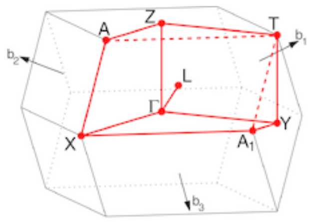
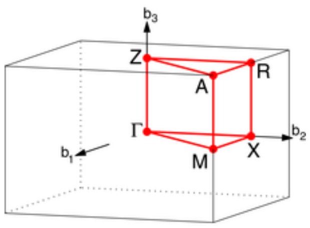
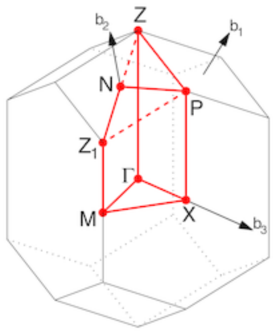
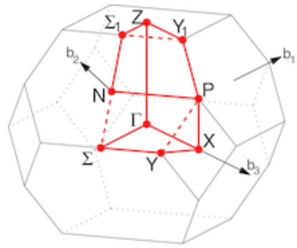
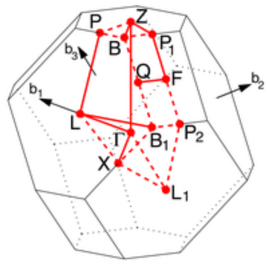
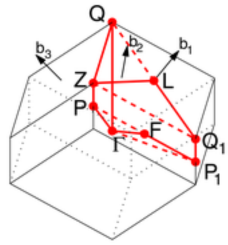

The Brillouin zone (purple) and the Irreducible Brillouin zone (red) for a hexagonal lattice.



First Brillouin zone of FCC lattice, a truncated octahedron, showing symmetry labels for high symmetry lines and points

Other lattices have different types of high-symmetry points. They can be found in the illustrations below.

Lattice system	Bravais lattice (Abbreviation)	Brillouin zone types[3]			
Triclinic	Primitive triclinic (TRI)	Triclinic Lattice type 1a (TRI1a) 	Triclinic Lattice type 1b (TRI1b) 	Triclinic Lattice type 2a (TRI2a) 	Tricl 
Monoclinic	Primitive monoclinic (MCL)	Monoclinic Lattice (MCL) 			
	Base-centered monoclinic (MCLC)	Base Centered Monoclinic Lattice type 1 (MCLC1) 	Base Centered Monoclinic Lattice type 2 (MCLC2) 	Base Centered Monoclinic Lattice type 3 (MCLC3) 	Base 4 (M 
Orthorhombic	Primitive orthorhombic (ORC)	Simple Orthorhombic Lattice (ORC) 			
	Base-centered orthorhombic (ORCC)	Base Centered Orthorhombic Lattice (ORCC) 			
	Body-centered	Body Centered Orthorhombic Lattice			

	orthorhombic **(ORCI)**	(ORCI)  ORCI path: Γ-X-L-T-W-R-X_1-Z-Γ-Y-S-W|L_1-Y|Y_1-Z [Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]		
	Face-centered orthorhombic **(ORCF)**	Face Centered Orthorhombic Lattice type 1 (ORCF1)  $ORCF_1$ path: Γ-Y-T-Z-Γ-X-A_1-Y|T-X_1|X-A-Z|L-Γ [Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]	Face Centered Orthorhombic Lattice type 2 (ORCF2)  $ORCF_2$ path: Γ-Y-C-D-X-Γ-Z-D_1-H-C|C_1-Z|X-H_1|H-Y|L-Γ [Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]	Face Centered Orthorhombic Lattice type 3 (ORCF3)  $ORCF_3$ path: Γ-Y-T-Z-Γ-X-A_1-Y|X-A-Z|L-Γ [Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]
Tetragonal	**Primitive tetragonal** **(TET)**	Simple Tetragonal Lattice (TET)  TET path: Γ-X-M-Γ-Z-R-A-Z|X-R|M-A [Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]		
	Body-centered Tetragonal **(BCT)**	Body Centered Tetragonal Lattice type 1 (BCT1)  BCT_1 path: Γ-X-M-Γ-Z-P-N-Z_1-M|X-P [Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]	Body Centered Tetragonal Lattice type 2 (BCT2)  BCT_2 Path: Γ-X-Y-Σ-Γ-Z-$Σ_1$-N-P-Y_1-Z|X-P [Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]	
Rhombohedral	**Primitive rhombohedral** **(RHL)**	Rhombohedral Lattice type 1 (RHL1)  RHL_1 path: Γ-L-B_1|B-Z-Γ-X|Q-F-P_1-Z|L-P [Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]	Rhombohedral Lattice type 2 (RHL2)  RHL_2 path: Γ-P-Z-Q-Γ-F-P_1-Q_1-L-Z [Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]	
Hexagonal	**Primitive hexagonal**	Hexagonal Lattice (HEX)		

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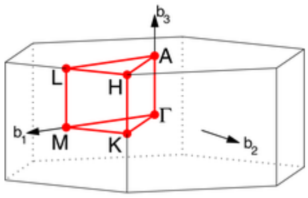
<tr><td></td><td>(HEX)</td><td>

HEX path: Γ-M-K-Γ-A-L-H-A|L-M|K-H
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]</td></tr>
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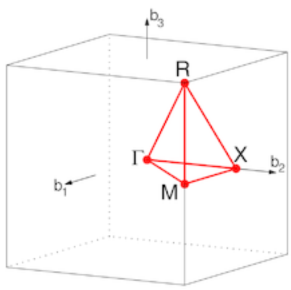
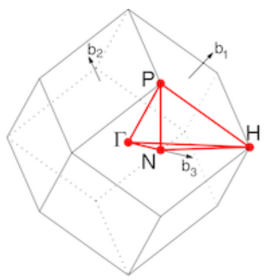
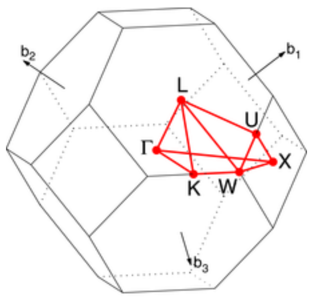
(CUB)</td><td>Simple Cubic Lattice (CUB)


CUB path: Γ-X-M-Γ-R-X|M-R
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]</td></tr>
<tr><td>Body-centered cubic
(BCC)</td><td>Body Centered Cubic Lattice (BCC)


BCC path: Γ-H-N-Γ-P-H|P-N
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]</td></tr>
<tr><td>Face-centered cubic
(FCC)</td><td>Face Centered Cubic Lattice (FCC)


FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]</td></tr>
</table>

See also

- Fundamental pair of periods
- Fundamental domain

References

1. "Topic 5-2: Nyquist Frequency and Group Velocity" (http://solidstate.mines.edu/videonotes/VN_5_2.pdf) (PDF). *Solid State Physics in a Nutshell*. Colorado School of Mines.
2. Ibach, Harald; Lüth, Hans (1996). *Solid-State Physics, An Introduction to Principles of Materials Science* (2nd ed.). Springer-Verlag. ISBN 978-3-540-58573-2.
3. Setyawan, Wahyu; Curtarolo, Stefano (2010). "High-throughput electronic band structure calculations: Challenges and tools". *Computational Materials Science*. **49** (2): 299–312. arXiv:1004.2974 (https://arxiv.org/abs/1004.2974). Bibcode:2010arXiv1004.2974S (https://ui.adsabs.harvard.edu/abs/2010arXiv1004.2974S). doi:10.1016/j.commatsci.2010.05.010 (https://doi.org/10.1016%2Fj.commatsci.2010.05.010).

Bibliography

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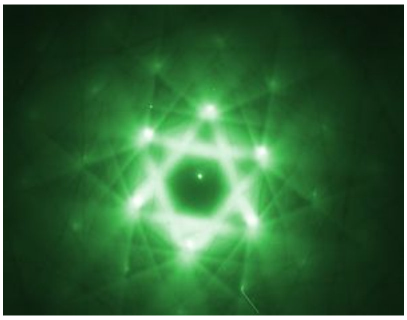
- Ashcroft, Neil W.; Mermin, N. David (1976). *Solid State Physics*. Orlando: Harcourt. ISBN 978-0-03-049346-1.
- Brillouin, Léon (1930). "Les électrons dans les métaux et le classement des ondes de de Broglie correspondantes" (http://gallica.bnf.fr/ark:/12148/bpt6k31445). *Comptes Rendus Hebdomadaires des Séances de l'Académie des Sciences*. **191** (292).



Brillouin-zone construction by selected area diffraction, using 300 keV electrons.

External links

- Brillouin Zone simple lattice diagrams by Thayer Watkins (http://www2.sjsu.edu/faculty/watkins/brillouin.htm)
- Brillouin Zone 3d lattice diagrams by Technion. (http://phycomp.technion.ac.il/~nika/brillouin_zones.html)
- DoITPoMS Teaching and Learning Package- "Brillouin Zones" (http://www.doitpoms.ac.uk/tlplib/brillouin_zones/index.php)
- Aflowlib.org consortium database (Duke University) (http://www.aflowlib.org)
- AFLOW Standardization of VASP/QUANTUM ESPRESSO input files (Duke University) (http://materials.duke.edu/awrapper.html)