MLL 100

Introduction to Materials Science and Engineering

Lecture-5

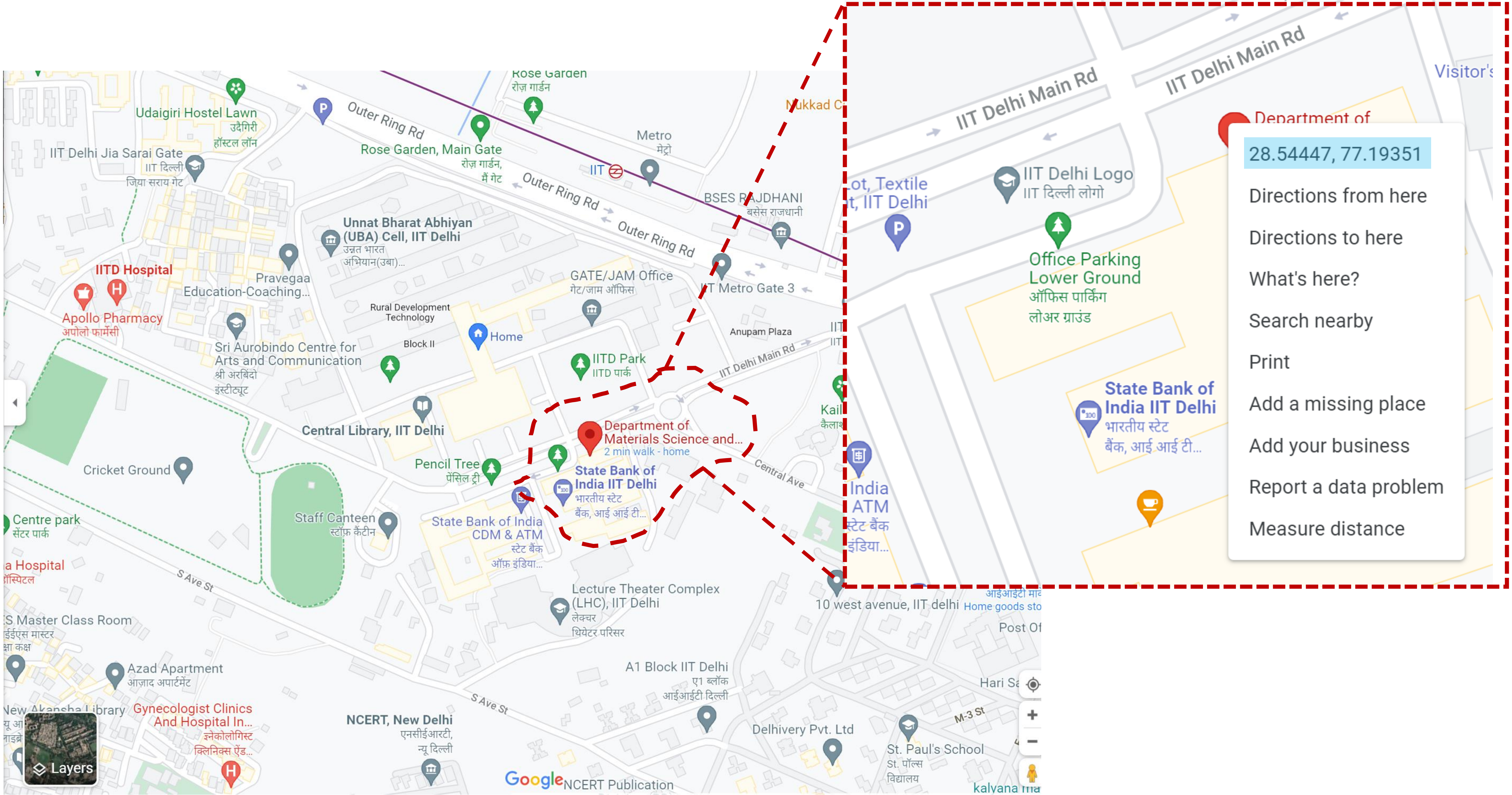
Dr. Sangeeta Santra (*ssantra@mse.iitd.ac.in*)

IIT Delhi
Department of Materials Science and Engineering

January 12, 2022

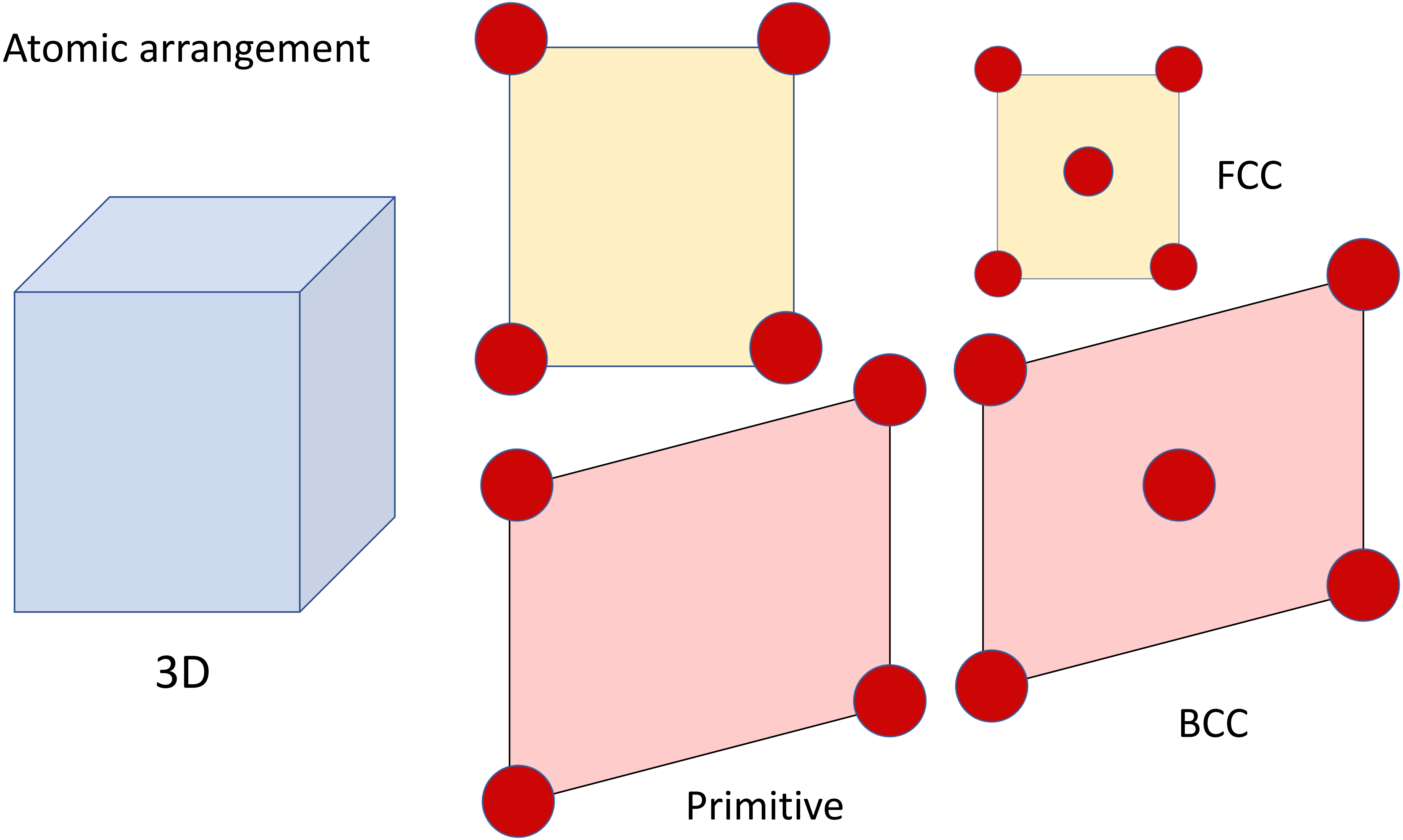
What we learnt in Lecture-4?

- Crystal
- Crystal systems
- Bravais lattices

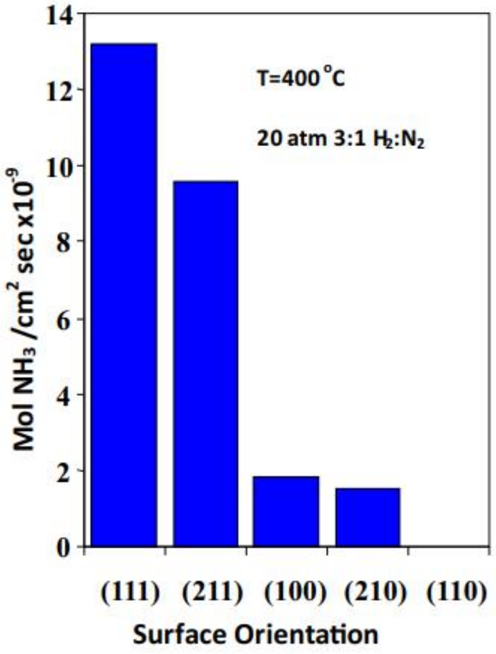


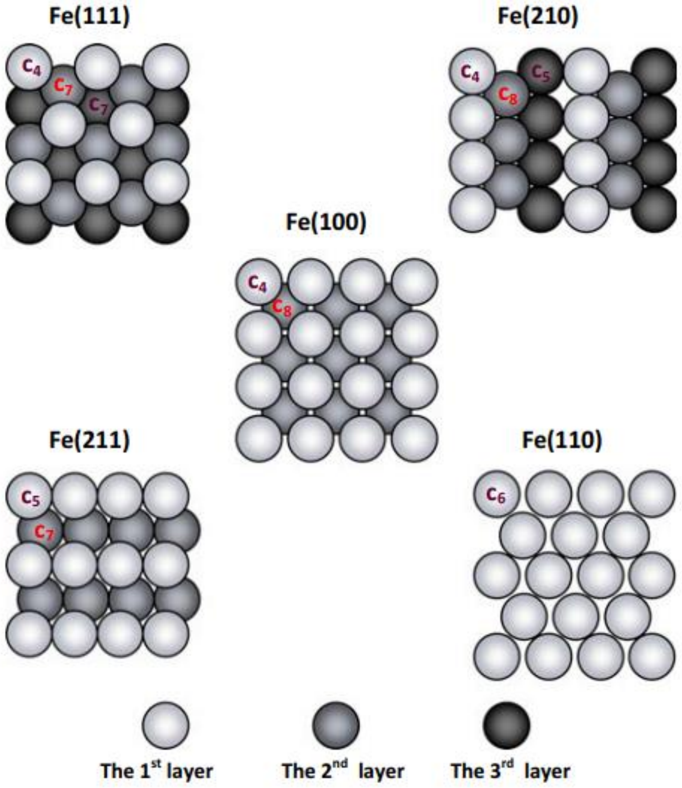
Udaigiri Hostel Lawn
उदैगिरी हॉस्टल लॉन
IIT Delhi Jia Sarai Gate
IIT दिल्ली जिया सराय गेट
Outer Ring Rd
Rose Garden, Main Gate
रोज़ गार्डन, मैं गेट
Rose Garden
रोज़ गार्डन
Metro
मेट्रो
IIT
BSES RAJDHANI
बसेस राजधानी
Unnat Bharat Abhiyan (UBA) Cell, IIT Delhi
उन्नत भारत अभियान(उबा)...
IITD Hospital
Pravegaa Education-Coaching...
Apollo Pharmacy
अपोलो फार्मेसी
GATE/JAM Office
गेट/जाम ऑफिस
IIT Metro Gate 3
Rural Development Technology
Block II
Home
Anupam Plaza
Sri Aurobindo Centre for Arts and Communication
श्री अरबिंदो इंस्टीट्यूट
IITD Park
IITD पार्क
IIT Delhi Main Rd
Central Library, IIT Delhi
Department of Materials Science and...
2 min walk - home
Cricket Ground
Pencil Tree
पेंसिल ट्री
State Bank of India IIT Delhi
भारतीय स्टेट बैंक, आई आई टी...
Central Ave
Centre park
सेंटर पार्क
Staff Canteen
स्टॉफ़ कैंटीन
State Bank of India CDM & ATM
स्टेट बैंक ऑफ़ इंडिया...
a Hospital
S Ave St
Lecture Theater Complex (LHC), IIT Delhi
लेक्चर थियेटर परिसर
10 west avenue, IIT delhi
Home goods sto
Post Of
S Master Class Room
Azad Apartment
आज़ाद अपार्टमेंट
A1 Block IIT Delhi
ए1 ब्लॉक आईआईटी दिल्ली
Hari Sa
New Akansha Library
Gynecologist Clinics And Hospital In...
गाइनोकोलॉजिस्ट क्लिनिक्स ऐंड...
NCERT, New Delhi
एनसीईआरटी, न्यू दिल्ली
Delhivery Pvt. Ltd
M-3 St
St. Paul's School
St. पॉल्स विद्यालय
Layers
Google
NCERT Publication
kalyana ma
Visitor's
Department of
28.54447, 77.19351
Directions from here
Directions to here
What's here?
Search nearby
Print
Add a missing place
Add your business
Report a data problem
Measure distance
IIT Delhi Logo
IIT दिल्ली लोगो
Office Parking Lower Ground
ऑफिस पार्किंग लोअर ग्राउंड
State Bank of India IIT Delhi
भारतीय स्टेट बैंक, आई आई टी...
India ATM

Atomic arrangement

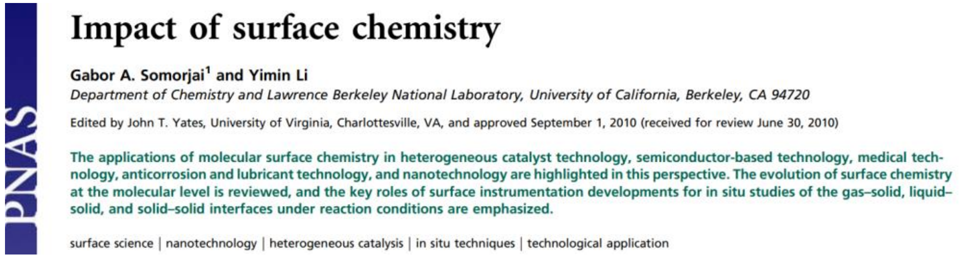


Reactivity of crystalline surfaces





(111) and (211) faces are the most reactive surfaces.


PNAS

Impact of surface chemistry

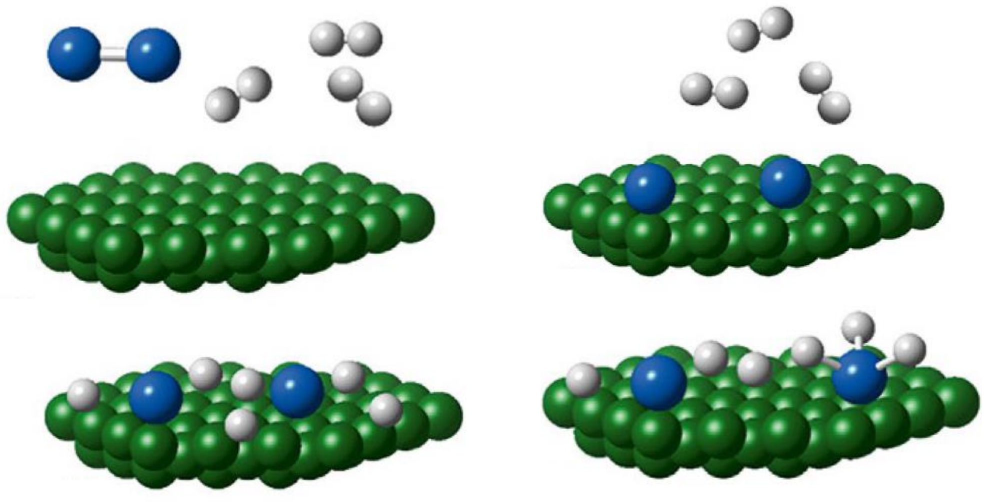
Gabor A. Somorjai[1] and Yimin Li

Department of Chemistry and Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720

Edited by John T. Yates, University of Virginia, Charlottesville, VA, and approved September 1, 2010 (received for review June 30, 2010)

The applications of molecular surface chemistry in heterogeneous catalyst technology, semiconductor-based technology, medical technology, anticorrosion and lubricant technology, and nanotechnology are highlighted in this perspective. The evolution of surface chemistry at the molecular level is reviewed, and the key roles of surface instrumentation developments for in situ studies of the gas–solid, liquid–solid, and solid–solid interfaces under reaction conditions are emphasized.

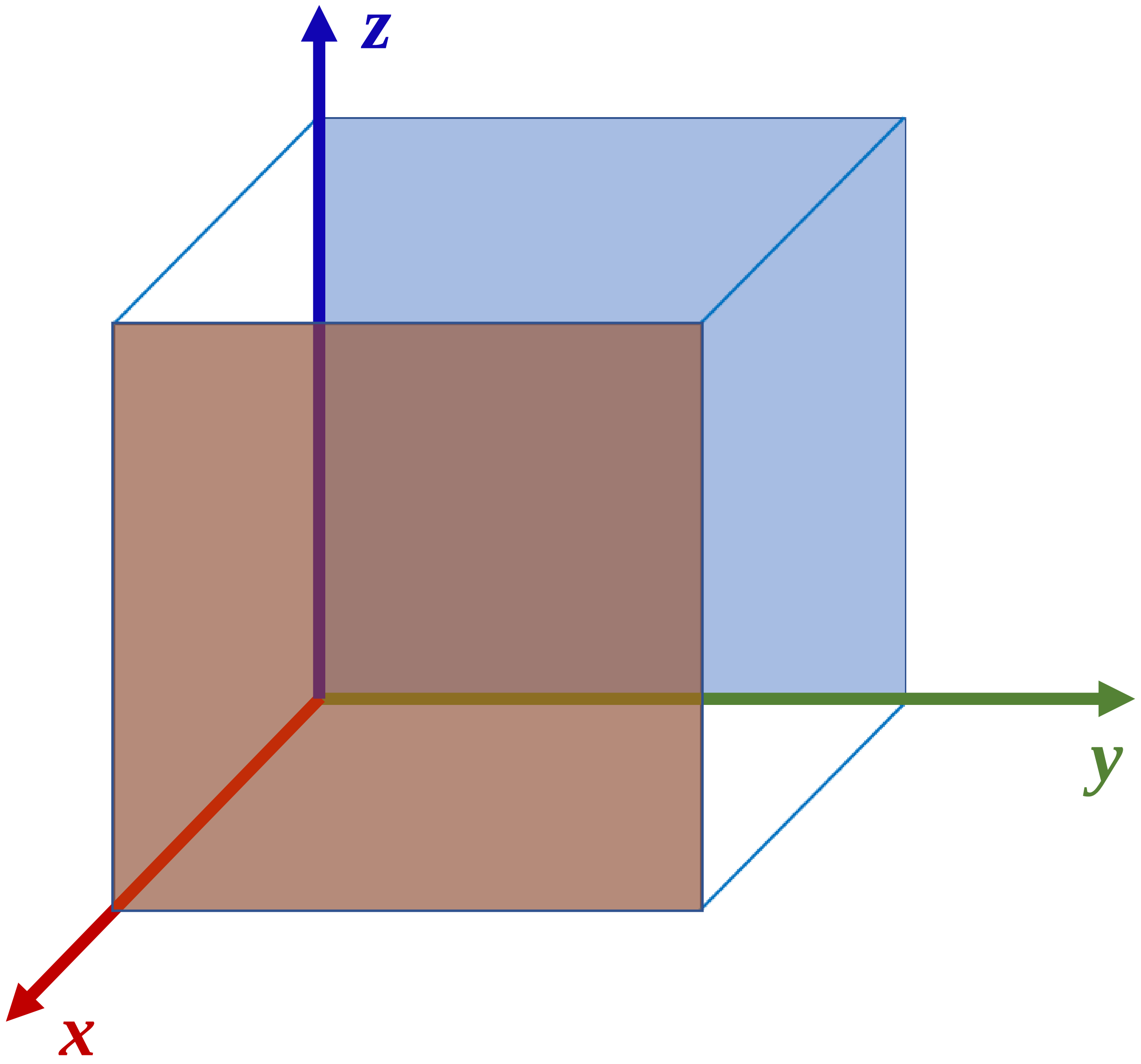
surface science | nanotechnology | heterogeneous catalysis | in situ techniques | technological application



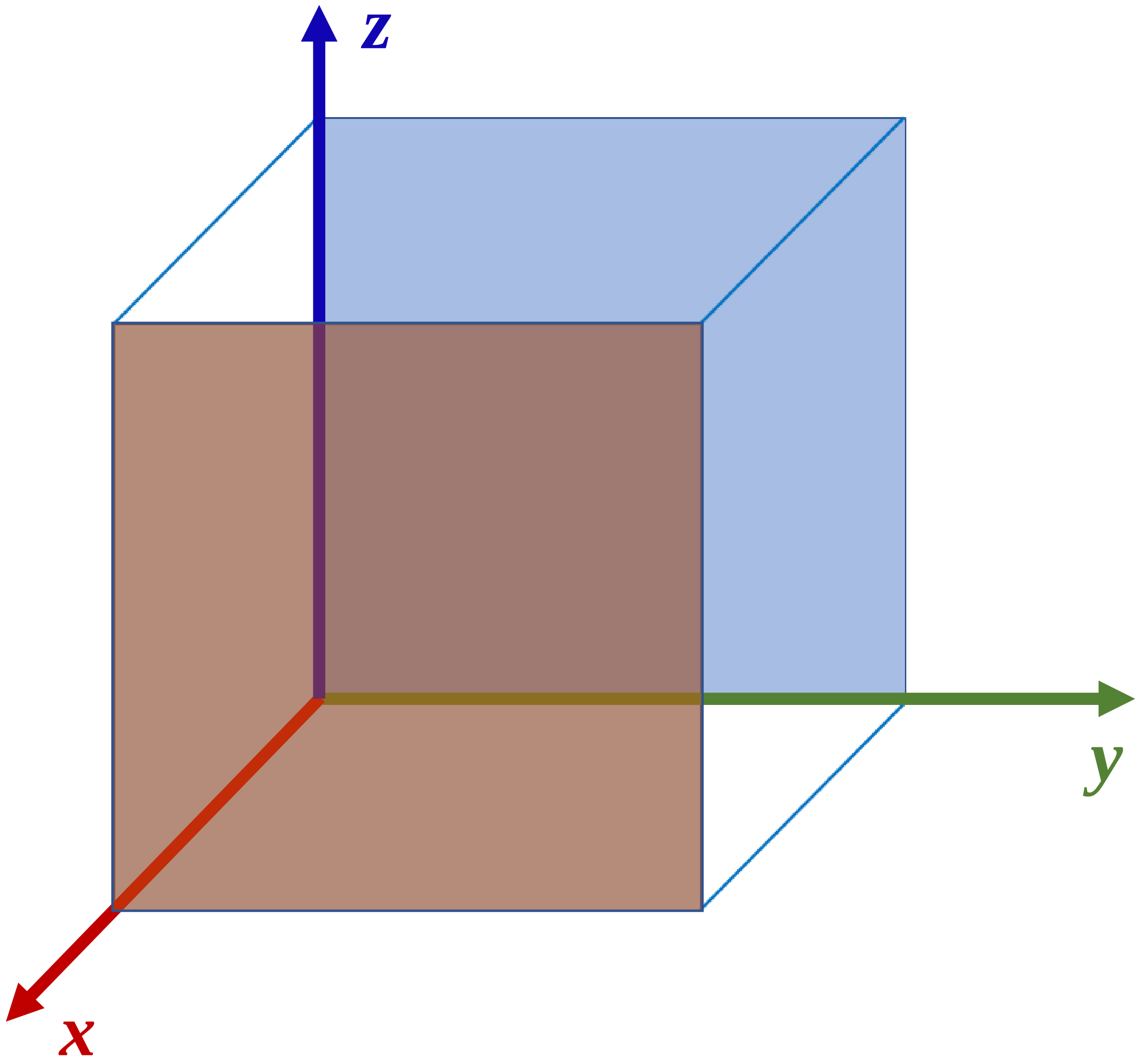
When do you tend to express your emotional reactivity?

Bonds decide the stability of a crystal --------> Understanding the bonds needs learning about the planes, directions and atomic arrangement

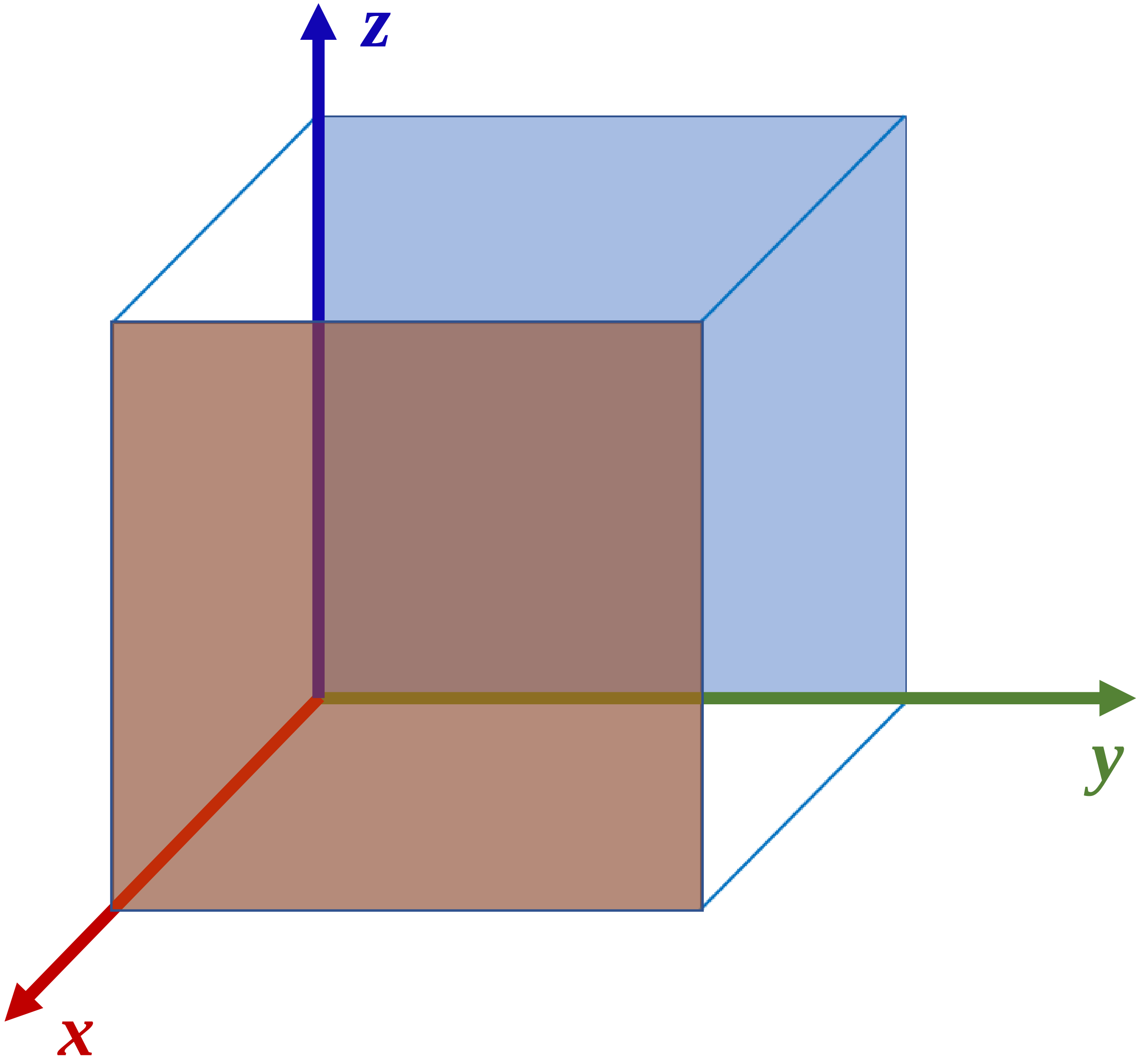
Miller indices ------ (Faces of a cube)



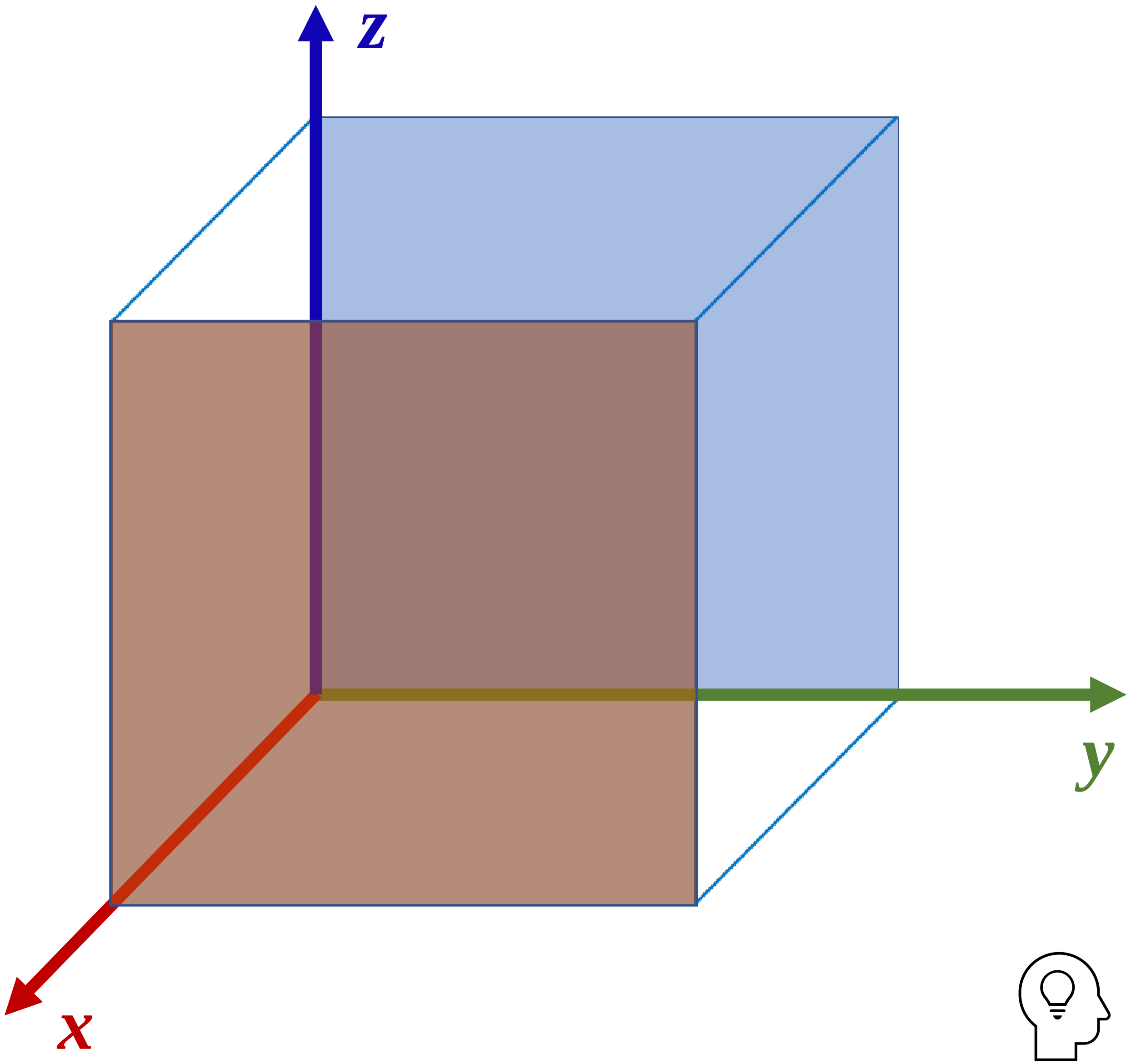
Miller indices ------ (Faces of a cube)



Miller indices ------ (Faces of a cube)

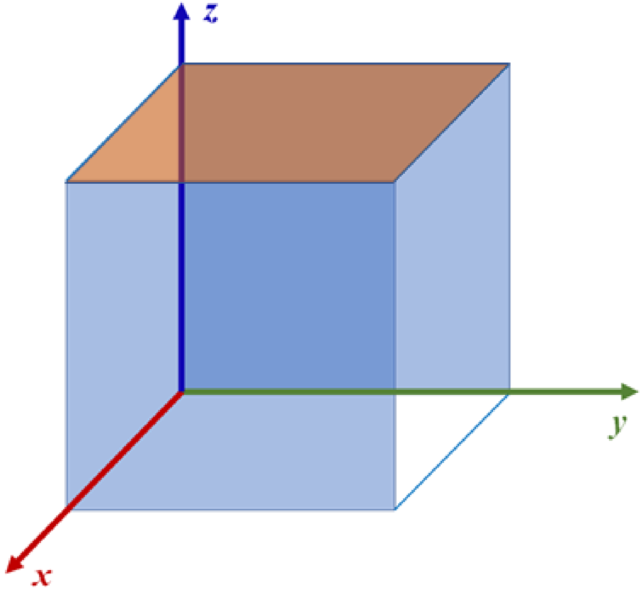


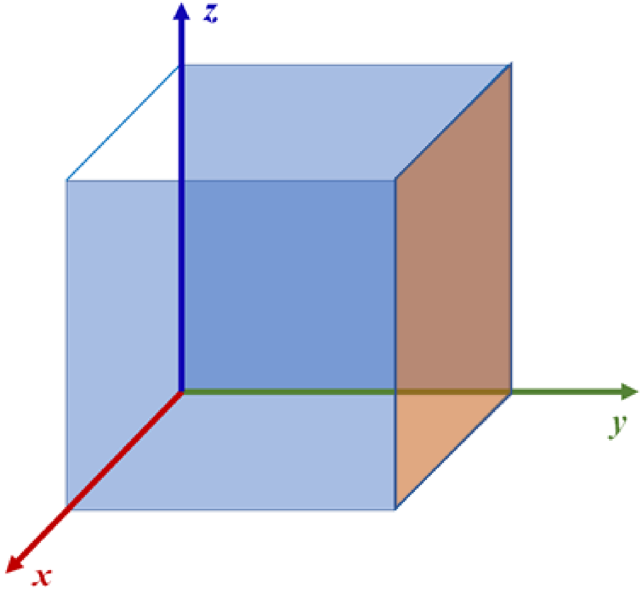
Miller indices ------ (Faces of a cube)



Intercepts	1	∞	∞
Reciprocals	$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{\infty}$
Plane	(100)		

Why do we not directly use the intercept form?



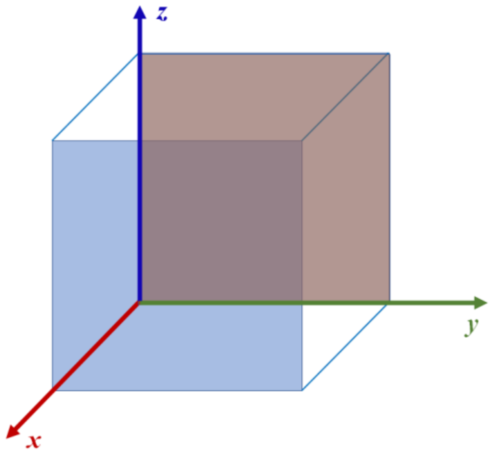


Intercepts	∞	∞	1
Reciprocals	$\frac{1}{\infty}$	$\frac{1}{\infty}$	$\frac{1}{1}$
Plane	(001)		

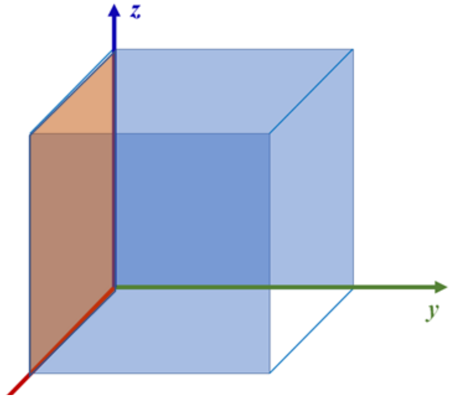
Intercepts	∞	1	∞
Reciprocals	$\frac{1}{\infty}$	$\frac{1}{1}$	$\frac{1}{\infty}$
Plane	(010)		

- Are these all equivalent planes ?
- Family of planes {100} --------- 6 in a cubic unit cell
- 4-fold rotational symmetry along the face normal.

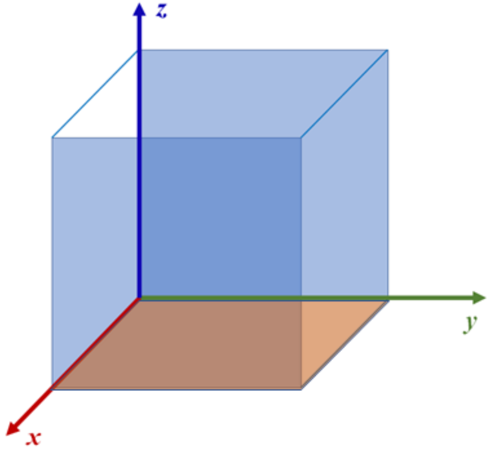
A set of planes related by symmetry operations of the lattice or the crystal is called a family of planes.



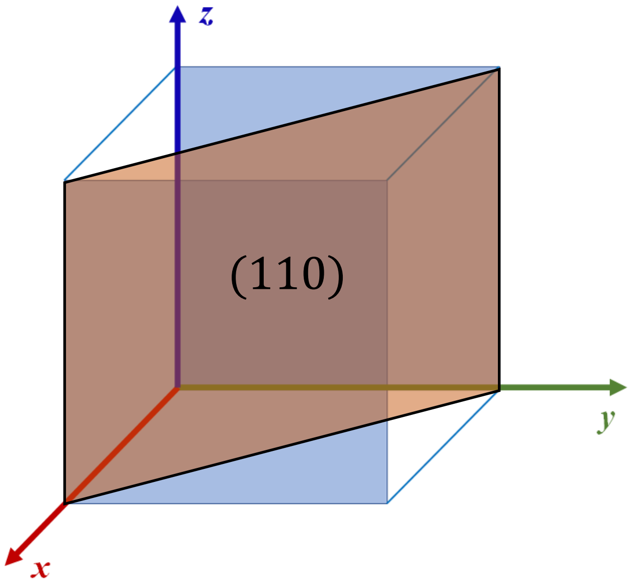
$(\bar{1}00)$

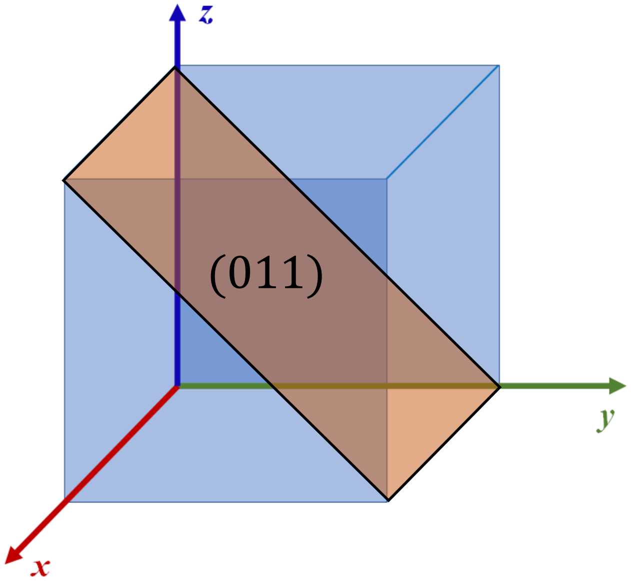


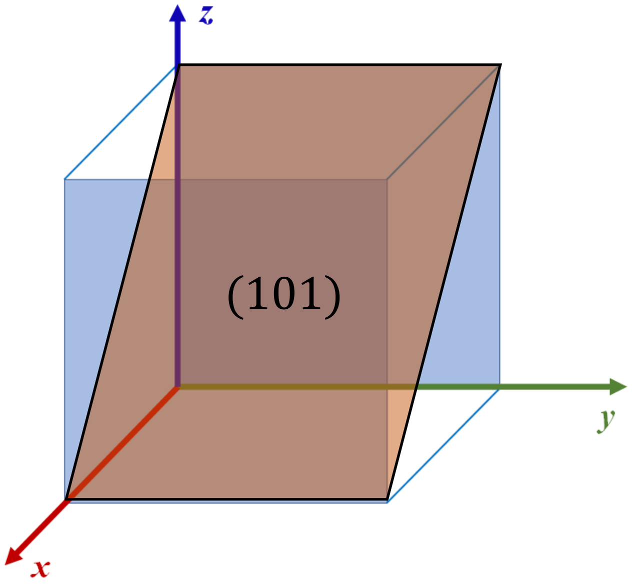
$(0\bar{1}0)$



$(00\bar{1})$

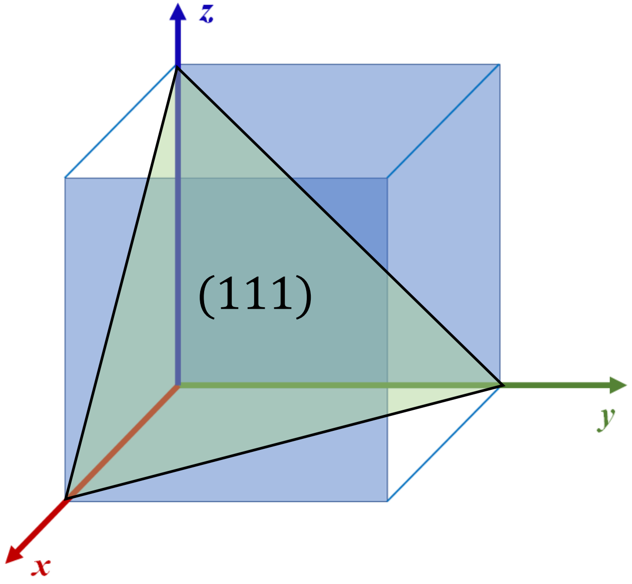


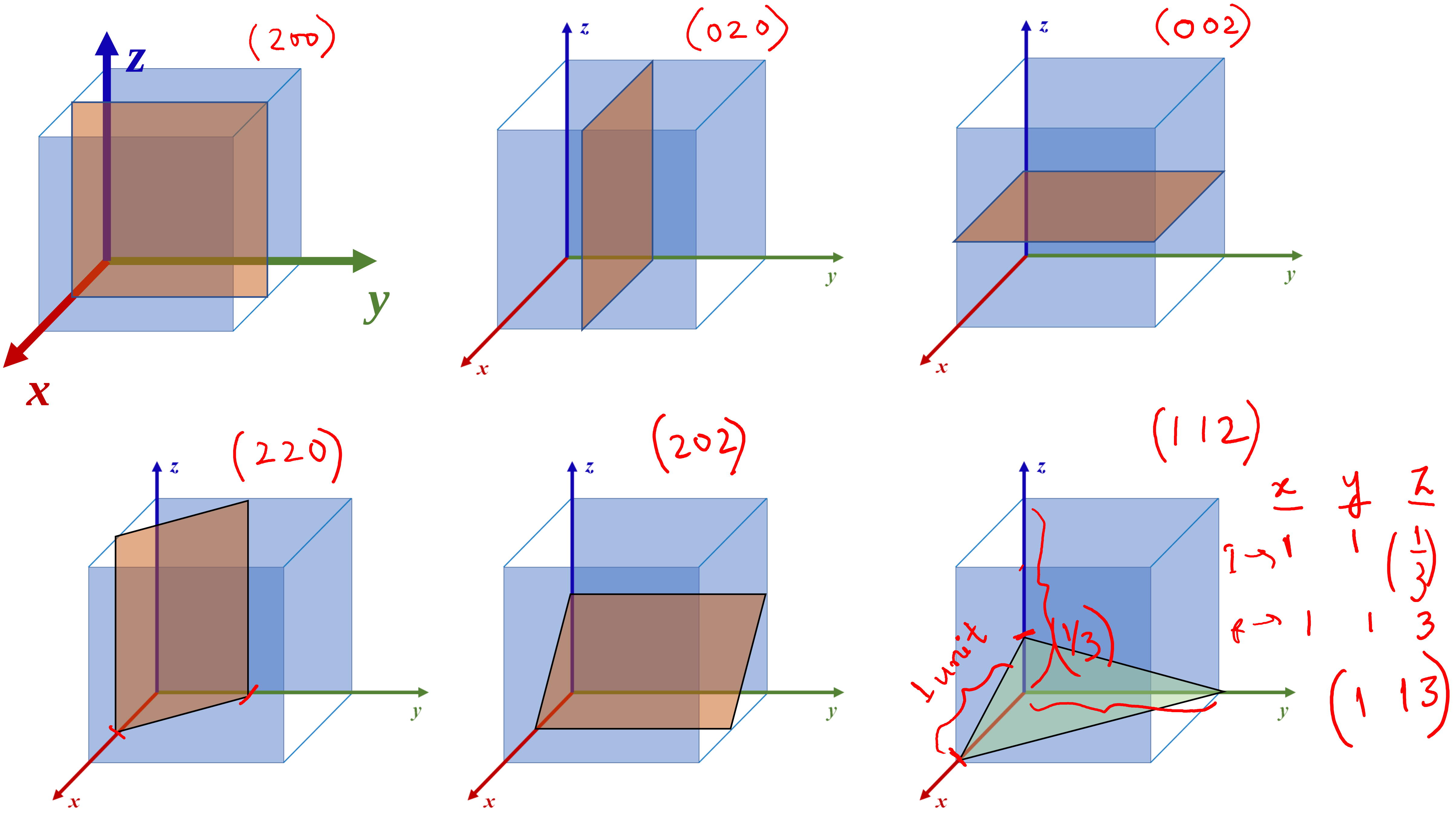




Intercepts	1	1	∞
Reciprocals	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{\infty}$
Plane		(110)	

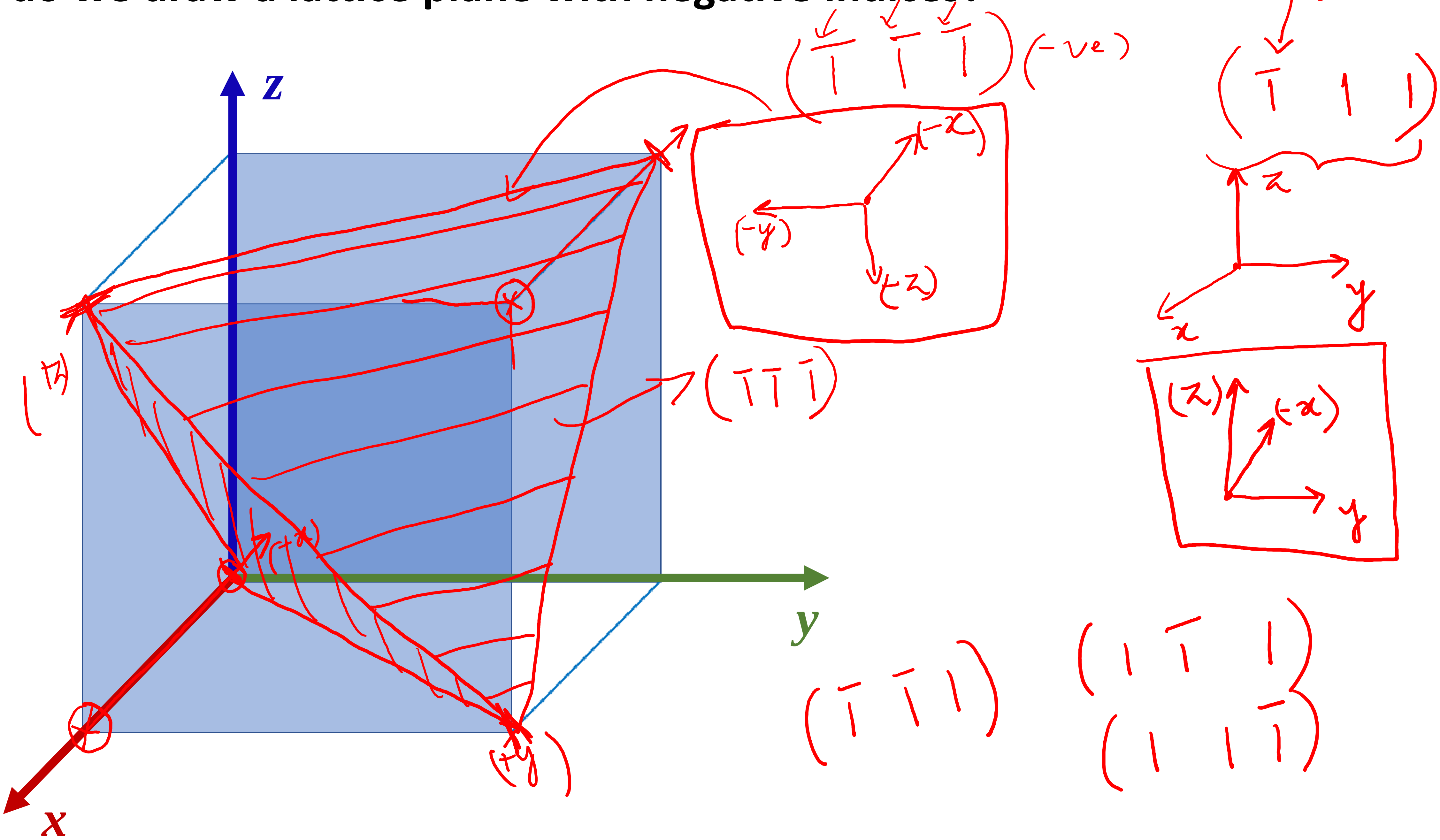
- Family of planes {110} --------- 6 in a cubic unit cell
- Family of planes {111} --------- 8 in a cubic unit cell





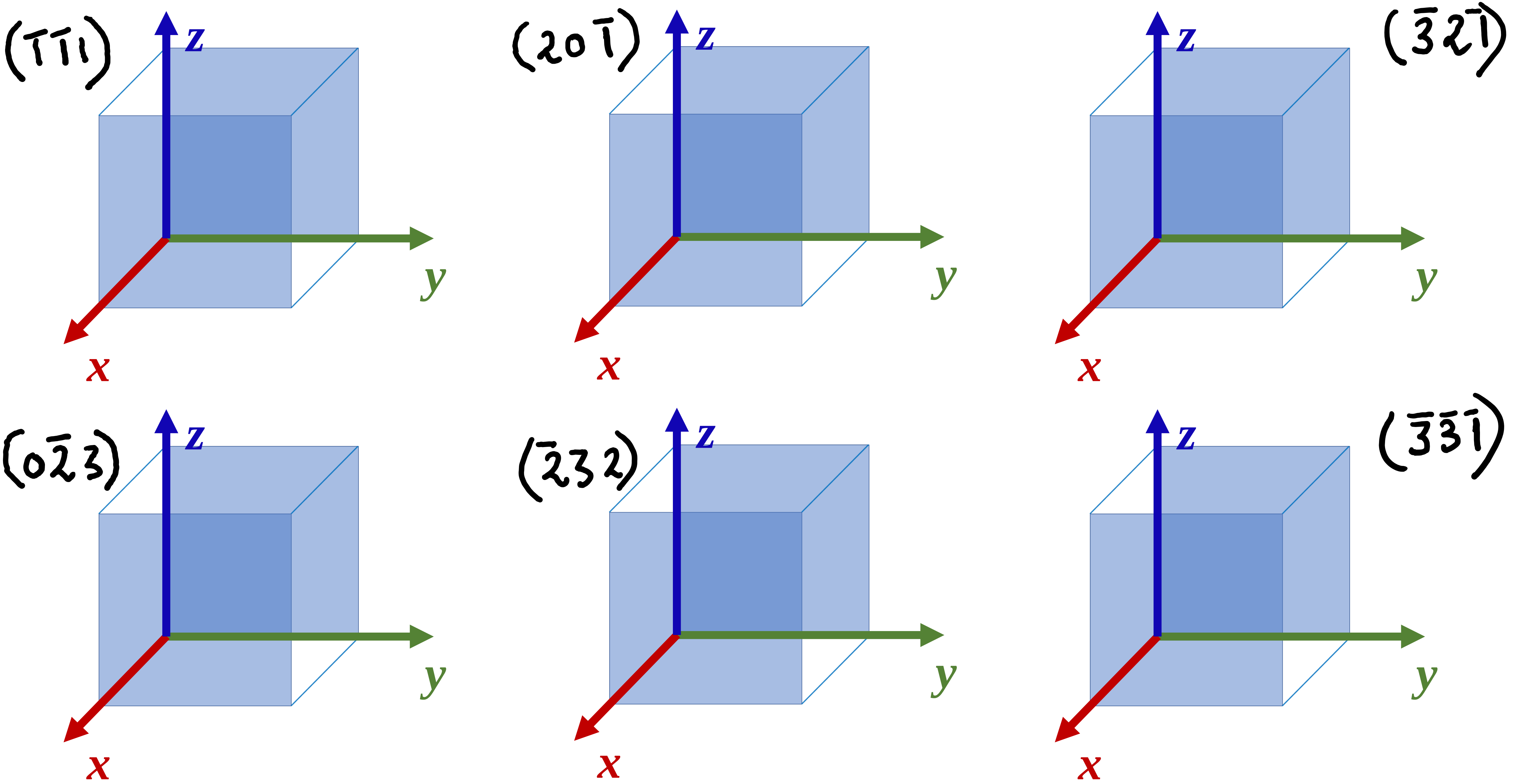
(200)
z
y
x
(020)
(002)
(220)
(202)
(112)
x y z
1→1 1 (1/3)
1 1 3
(1 1 3)
1 unit
1/3

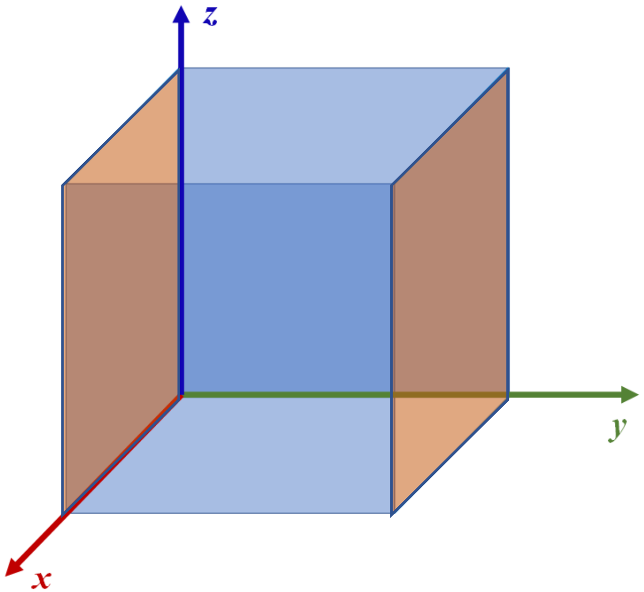
How do we draw a lattice plane with negative indices?

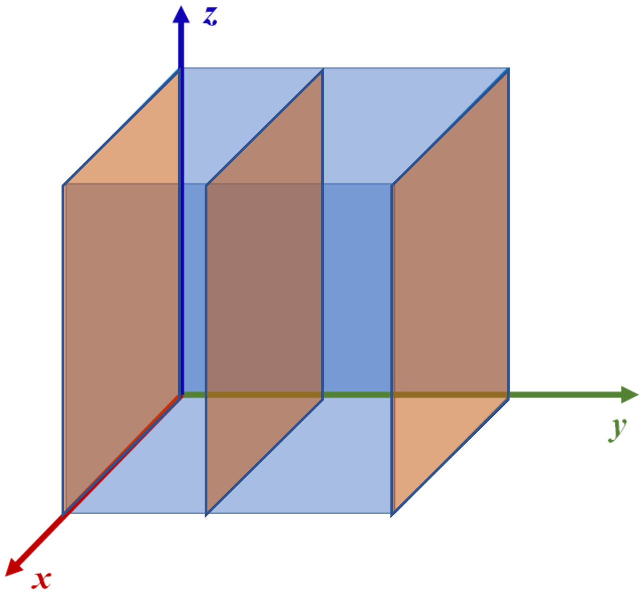


$(\bar{1}\;\bar{1}\;1)$ $(1\;\bar{1}\;1)$ $(1\;1\;\bar{1})$

How do we construct the lattice planes with the given Miller indices?







- Higher the indices are, smaller is the distance between the two adjacent planes.

- Distance between two lattice planes:
  Interplanar distance (d-spacing)

$$\boxed{\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}=\frac{1}{(d_{hkl})^2}}$$

$$\boxed{d_{hkl}=\frac{a}{\sqrt{h^2+k^2+l^2}}}$$

Volume and interplanar spacing

The following equations give the volume V of the unit cell.

Cubic: $V = a^3$

Tetragonal: $V = a^2 c$

Hexagonal: $V = \frac{\sqrt{3}\, a^2 c}{2} = 0.866 a^2 c$

Rhombohedral: $V = a^3 \sqrt{1 - 3\cos^2\alpha + 2\cos^3\alpha}$

Orthorhombic: $V = abc$

Monoclinic: $V = abc \sin\beta$

Triclinic: $V = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$

Interplanar spacing

The spacing d between adjacent (hkl) lattice planes is given by:

- Cubic:

$$\frac{1}{d^2} = \frac{h^2+k^2+l^2}{a^2}$$

- Tetragonal:

$$\frac{1}{d^2} = \frac{h^2+k^2}{a^2} + \frac{l^2}{c^2}$$

- Hexagonal:

$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2+hk+k^2}{a^2}\right) + \frac{l^2}{c^2}$$

- Rhombohedral:

$$\frac{1}{d^2} = \frac{(h^2+k^2+l^2)\sin^2\alpha + 2(hk+kl+hl)(\cos^2\alpha - \cos\alpha)}{a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$$

- Orthorhombic:

$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

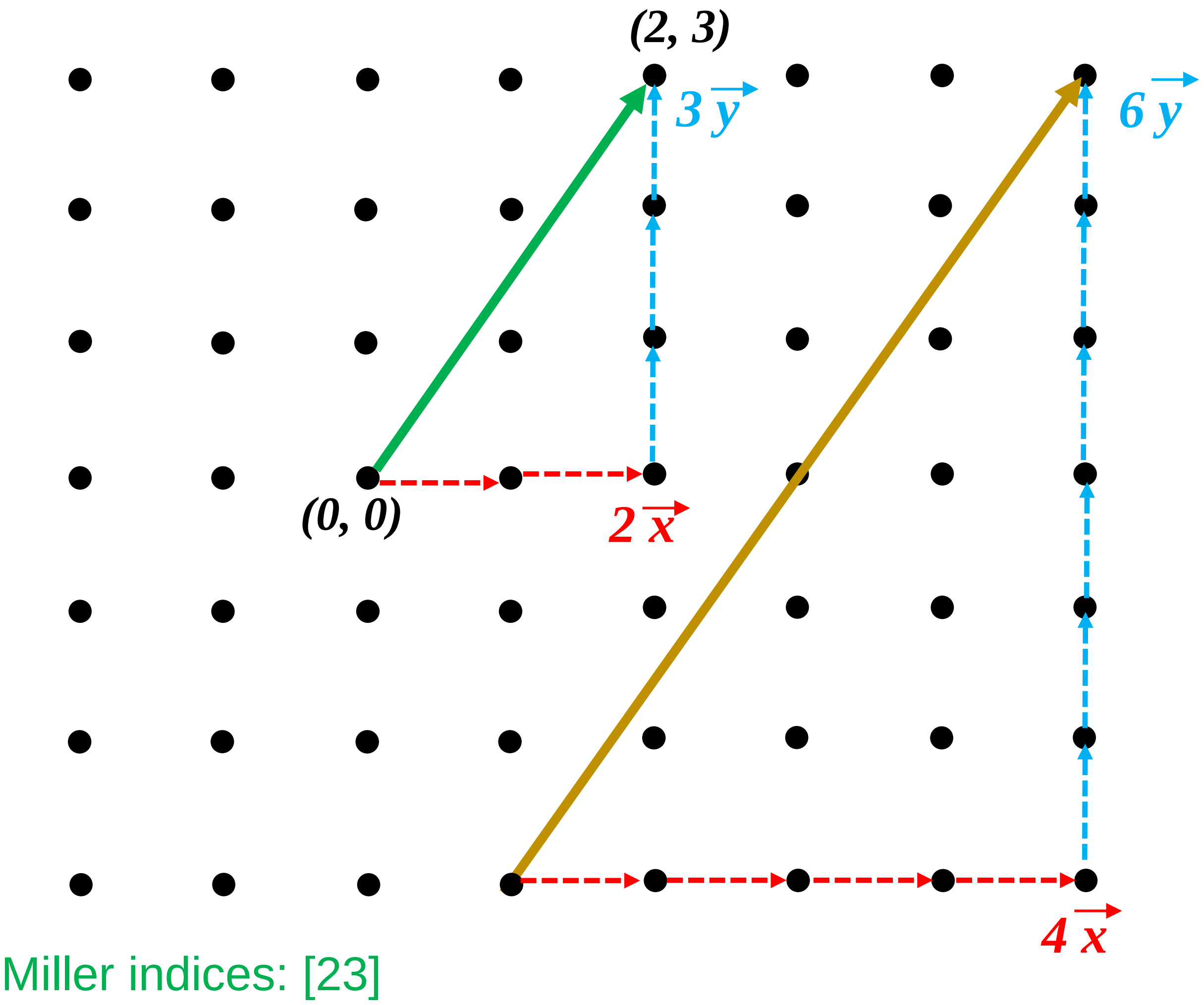
- Monoclinic:

$$\frac{1}{d^2} = \left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right)\csc^2\beta$$

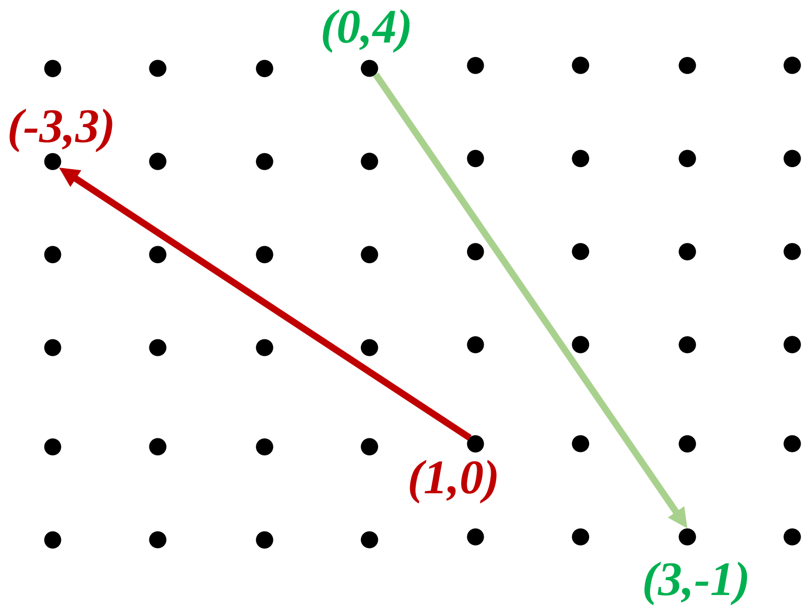
- Triclinic:

$$\frac{1}{d^2} = \frac{\frac{h^2}{a^2}\sin^2\alpha + \frac{k^2}{b^2}\sin^2\beta + \frac{l^2}{c^2}\sin^2\gamma}{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$$

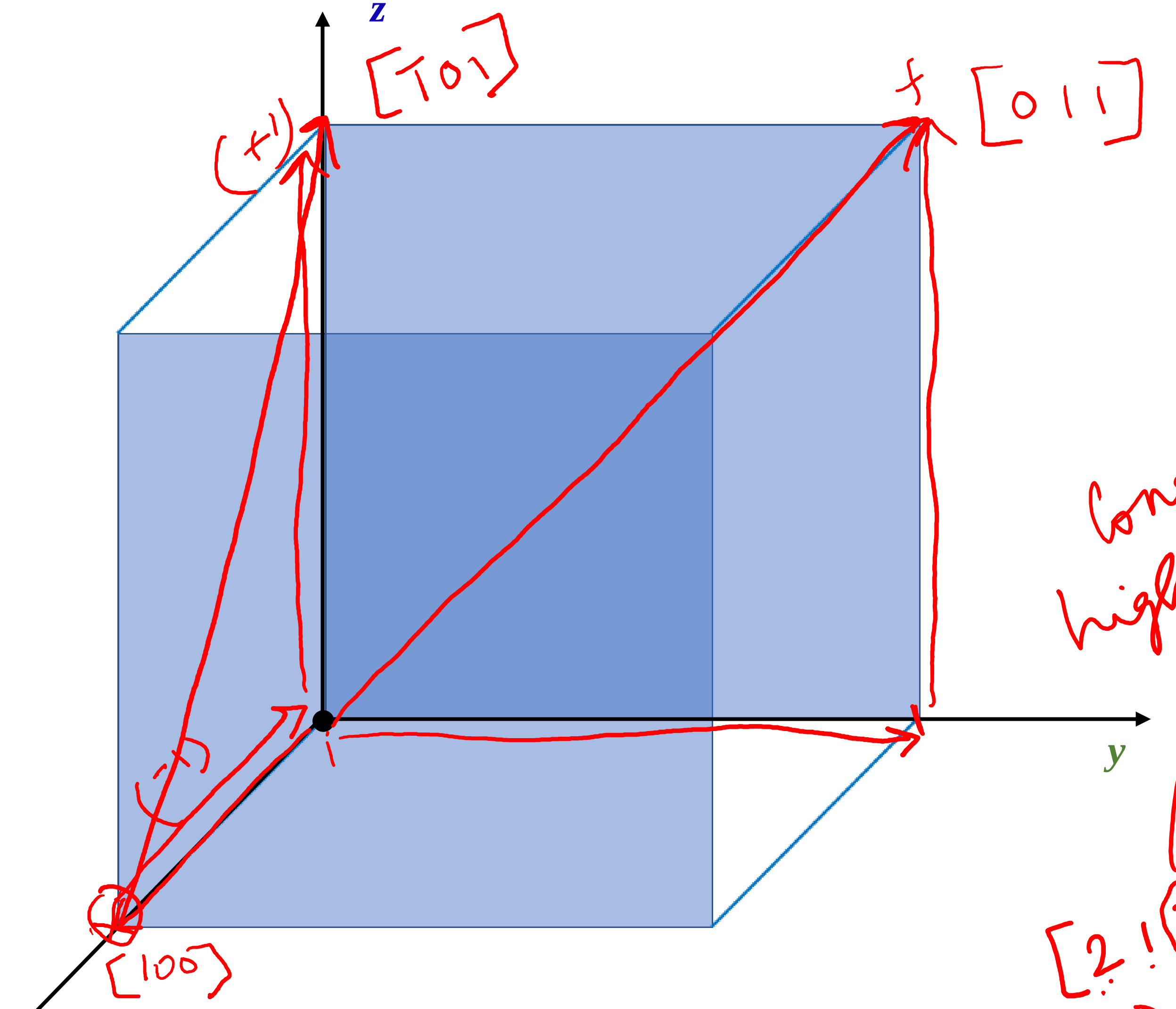
Miller indices for directions in 2-D

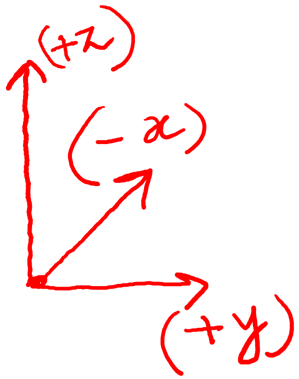


- Does the miller index for a direction necessarily start and end at distinct lattice points?



How to draw a direction if Miller indices are given?





[100]
[011]
[$\bar{1}$01]
[$\bar{2}$13]

[2 0 0]

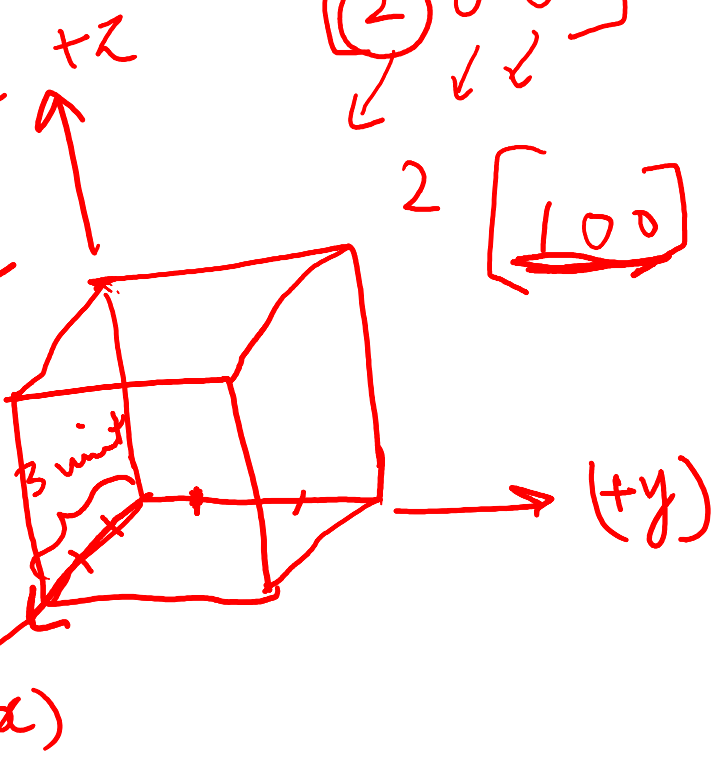
2 [1 0 0]

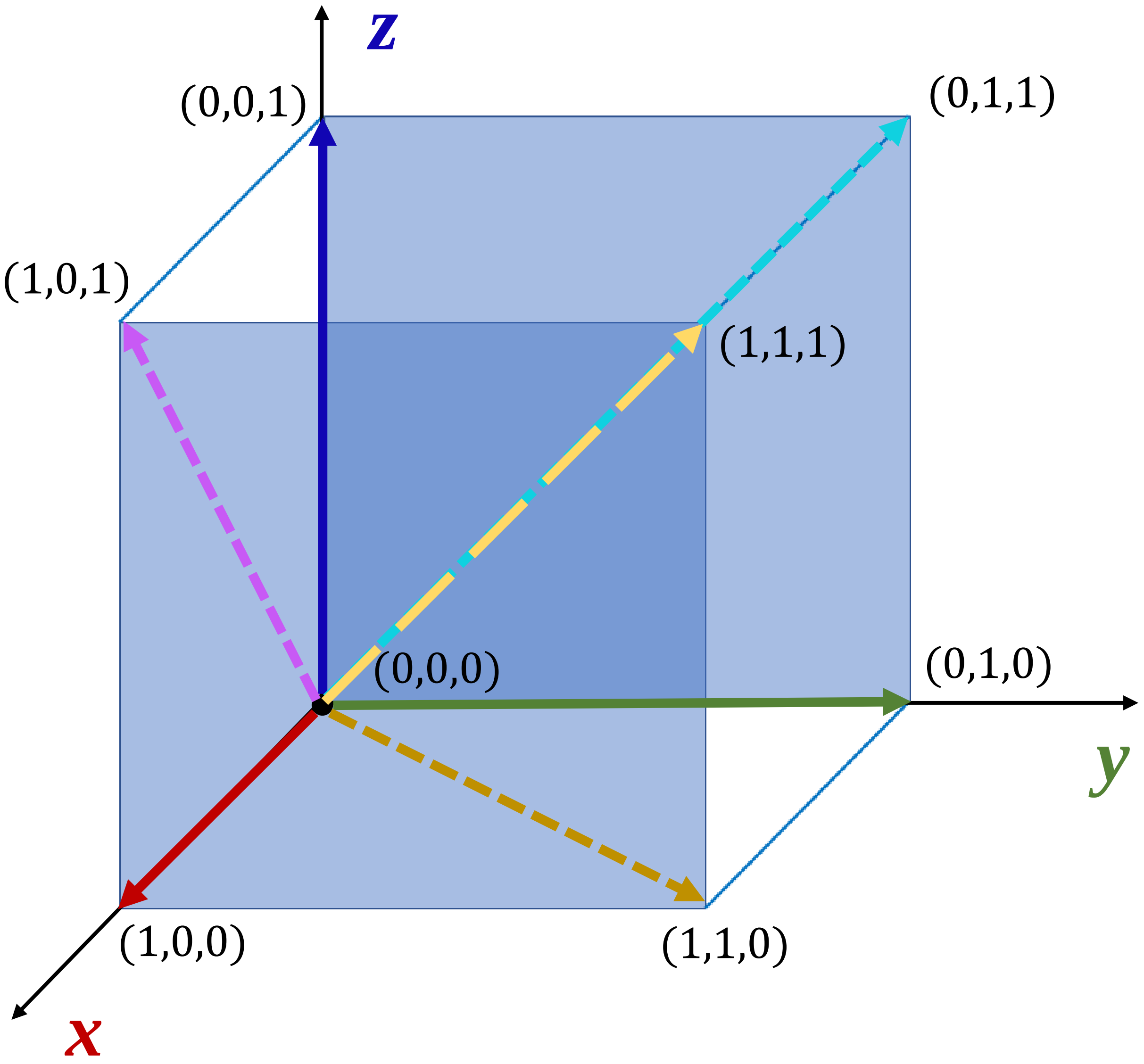
Consider the highest index value as your edge unit

Direction

[2 1 3]

$\left(\frac{2}{3}\right) \left(\frac{1}{3}\right) \left(\frac{3}{3}\right)$





[1 0 0]
[0 1 0]
[0 0 1]

Family of directions: <1 0 0>

[1 1 0]
[0 1 1]
[1 0 1]

Face diagonals
Family of directions: <1 1 0>

[1 1 1]

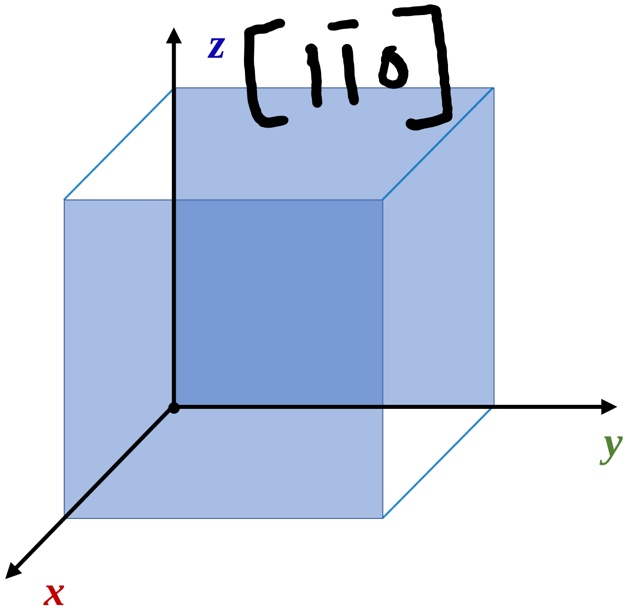
Body diagonal

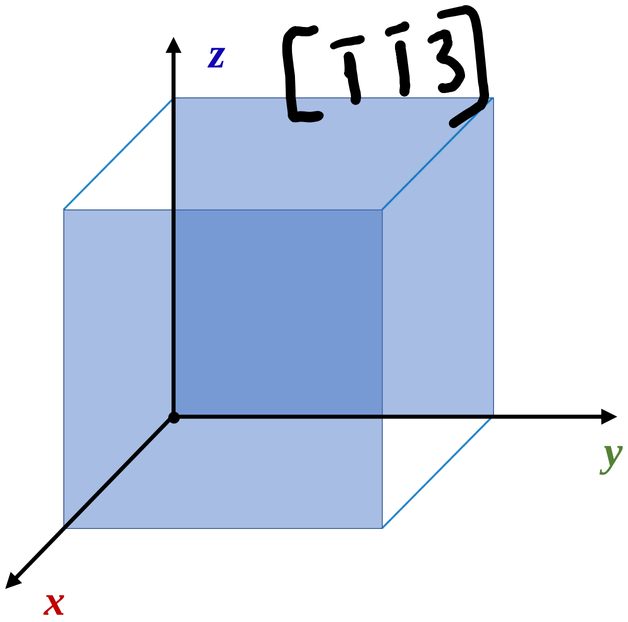
Family of directions

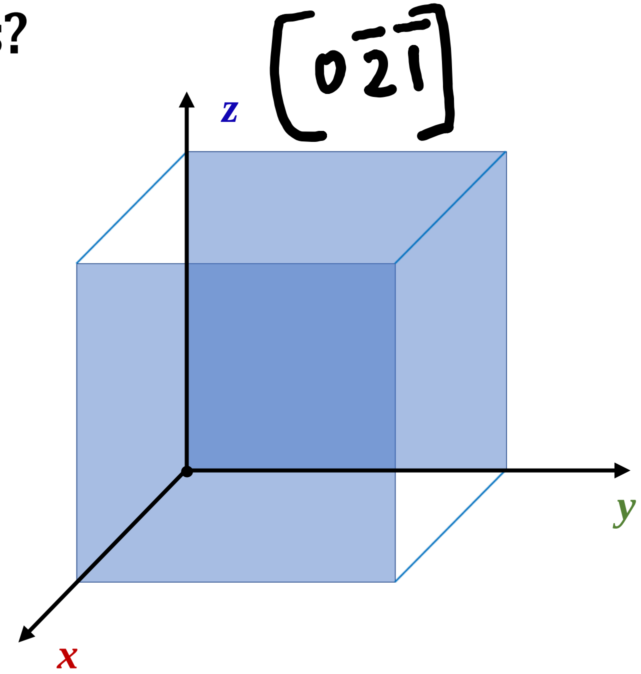
Index	Members in family for cubic lattices	Number
<100>	$[100],[\bar{1}00],[0\bar{1}0],[001],[00\bar{1}]$	3 x 2 = 6
<110>	$[110],[\bar{1}10],[1\bar{1}0],[\bar{1}\bar{1}0],[101],[\bar{1}01],[10\bar{1}],[\bar{1}0\bar{1}],[011],[0\bar{1}1],[01\bar{1}],[0\bar{1}\bar{1}]$	6 x 2 = 12
<111>	$[111],[\bar{1}11],[1\bar{1}1],[11\bar{1}],[\bar{1}\bar{1}1],[\bar{1}1\bar{1}],[1\bar{1}\bar{1}],[\bar{1}\bar{1}\bar{1}]$	4 x 2 = 8

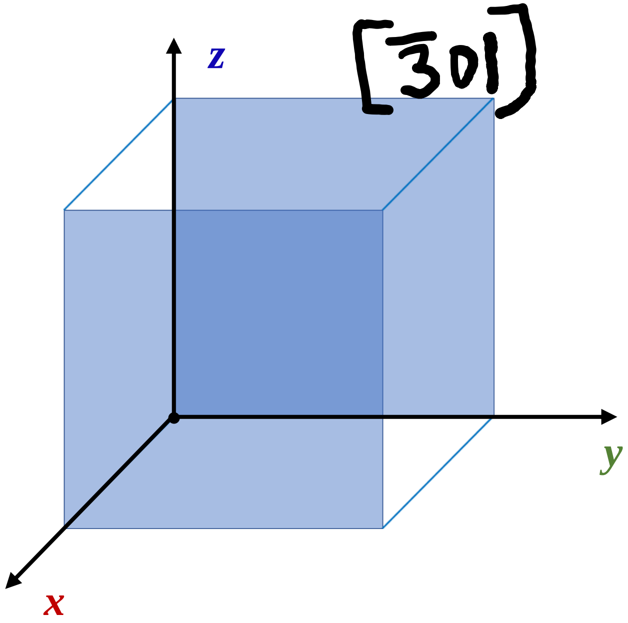
Symbol	Alternate symbol		
[ ]		→	Particular direction
< >	[[ ]]	→	Family of directions

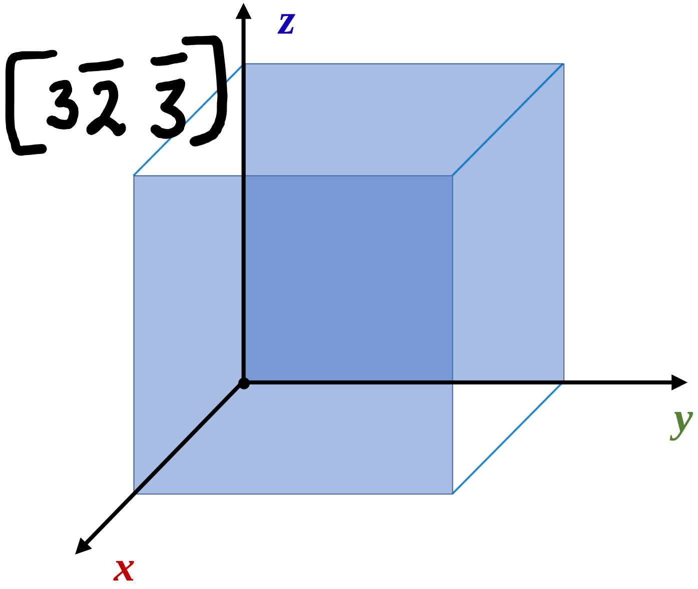
How do we construct the lattice directions with the given Miller indices?

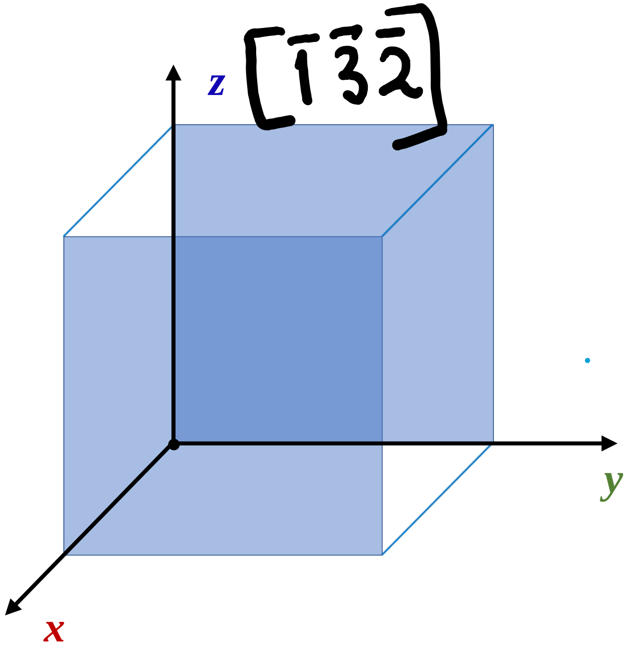


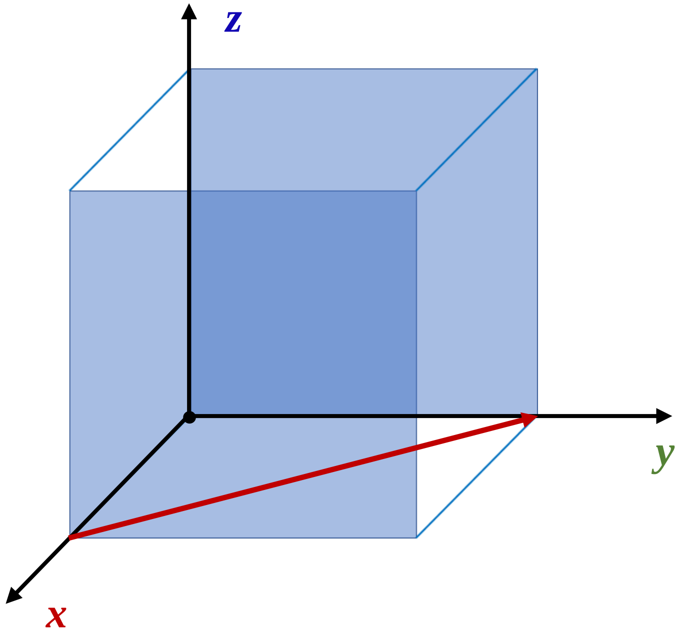


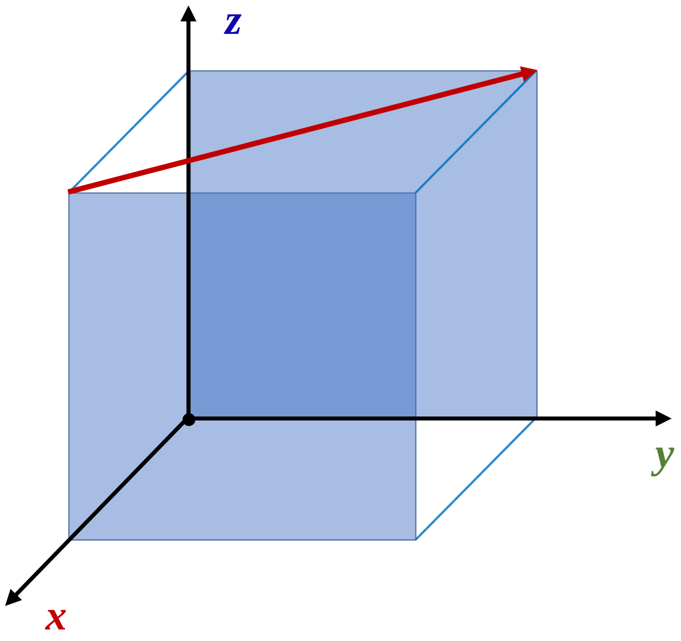


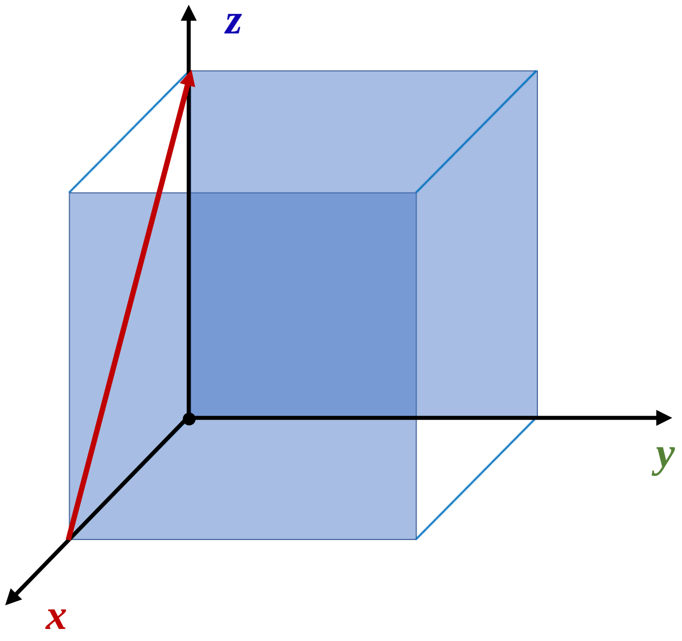


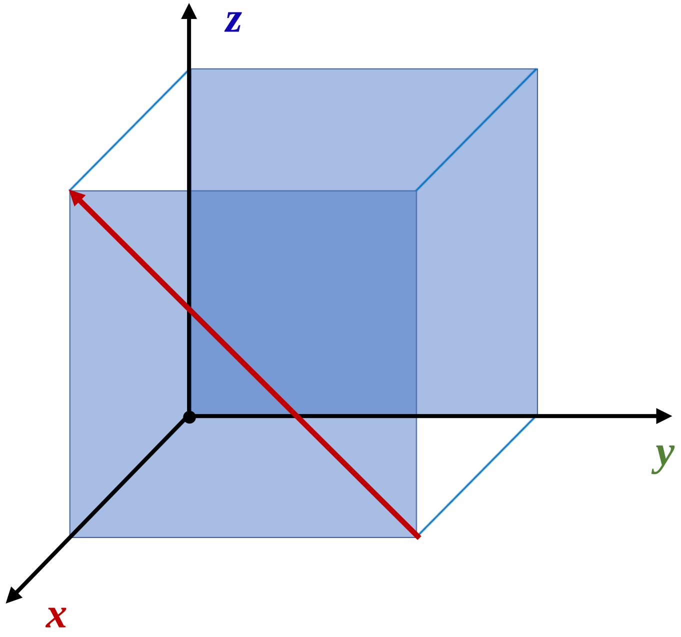


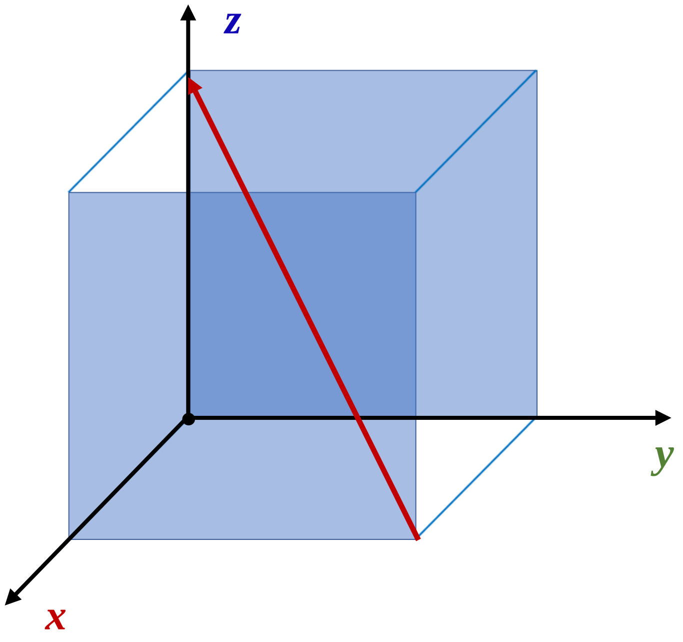


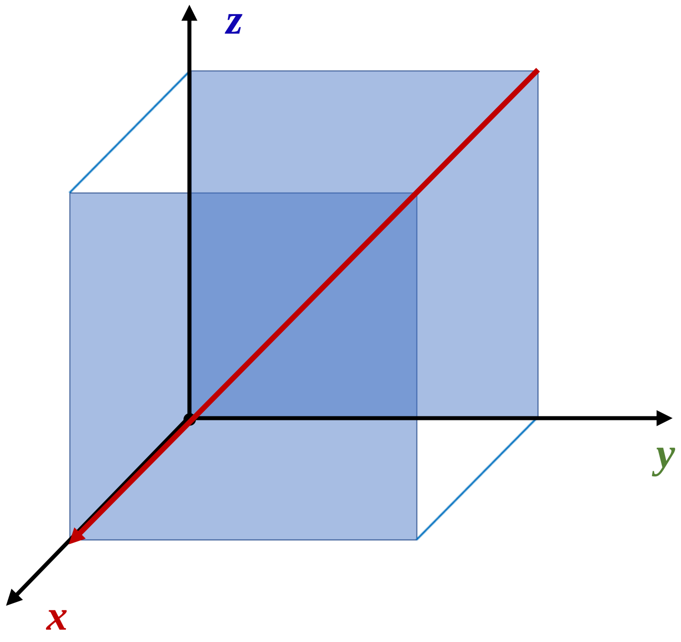

z
y
x


z
y
x


z
y
x


z
y
x


z
y
x


z
y
x