to parents

Welcome to 3.091

Lecture 16

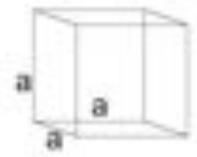
October 16, 2009

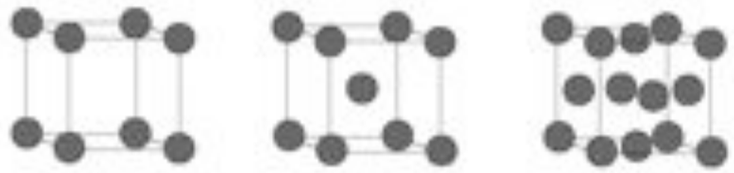
Crystallographic Notation & X-Rays

7 Crystal systems

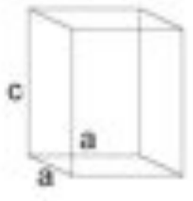
14 Bravais Lattices

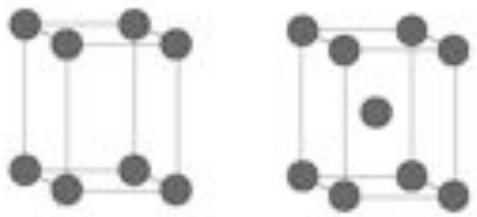
cubic
a=b=c
$\alpha=\beta=\gamma=90^o$



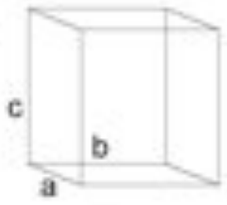


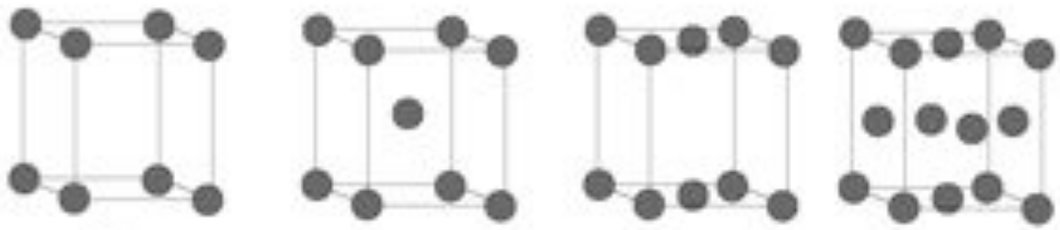
tetragonal
a=b≠c
$\alpha=\beta=\gamma=90^o$





orthorhombic
a≠b≠c
$\alpha=\beta=\gamma=90^o$

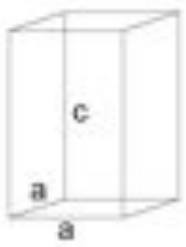


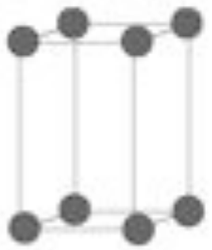


rhombohedral
a=b=c

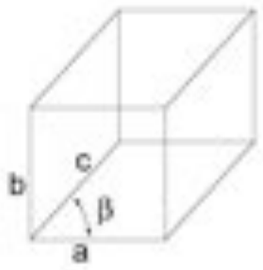
$\alpha=\beta=\gamma\neq90^o$

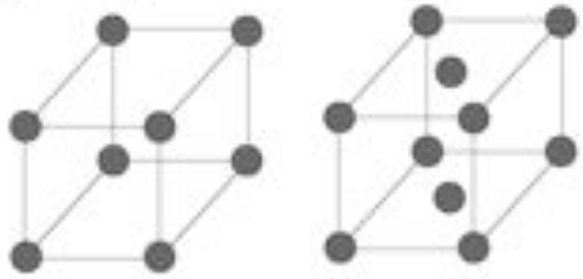
hexagonal
a=b≠c
$\alpha=\beta=90^o$
$\gamma=120^o$





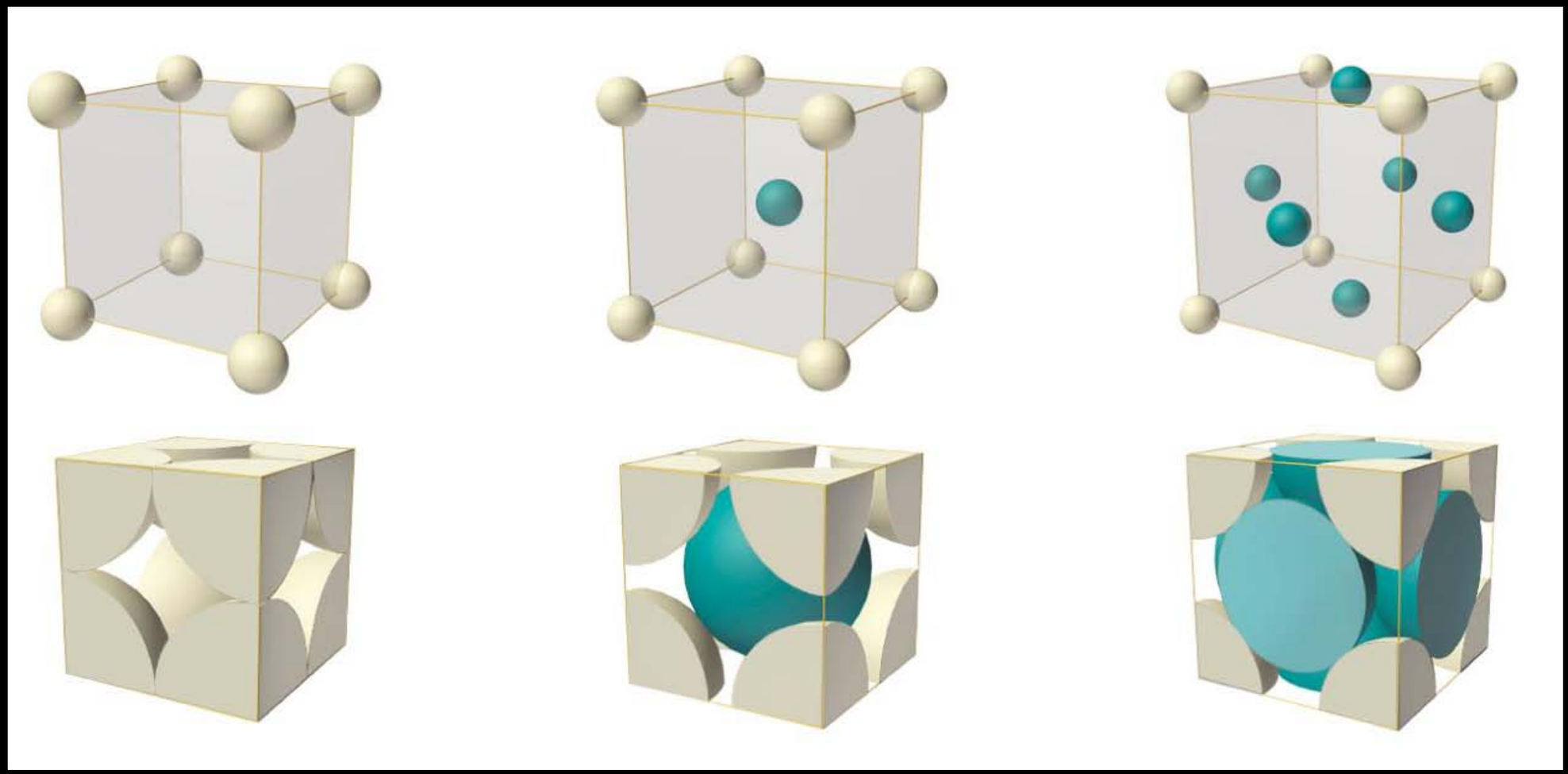
monoclinic
a≠b≠c
$\alpha=\gamma=90^o\neq\beta$





triclinic
a≠b≠c
$\alpha\neq\beta\neq\gamma\neq90^o$


ADMIRAL HOTEL



Averill, B., and P. Eldredge. *Chemistry: Principles, Patterns, and Applications*. Flat World Knowledge, 2011. ISBN: 9781453331224.

TABLE II. Characteristics of Cubic Lattices

	Simple	Body-Centered	Face-Centered
Unit Cell Volume	a^3	a^3	a^3
Lattice Points Per Cell	1	2	4
Nearest Neighbor Distance	a	$\frac{a\sqrt{3}}{2}$	$\frac{a}{\sqrt{2}}$
Number of Nearest Neighbors	6	8	12
Second Nearest Neighbor Distance	$a\sqrt{2}$	a	a
Number of Second Neighbors	12	6	6
a = f(r)	**2r**	**4r/√3**	**2√2r**
or 4r =	**√4 a**	**√3 a**	**√2 a**
packing density	**0.52**	**0.68**	**0.74**

Crystallographic Notation

position: x,y,z, coordinates, sep^{d} by commas, no enclosure
O: 0,0,0 **A**: 0,1,1 **B**: 1,0, ½

direction: move coordinate axes so that line passes through origin
- define vector from **O** to point on the line
- choose smallest set of integers
- no commas, enclose in brackets, clear fractions

$\xrightarrow[OB]{}$ 1 0 ½ clear fractions ☞ [201]

$\xrightarrow[AO]{}$ $[0\bar{1}\bar{1}]$ minus denoted by macron

can denote entire family of directions by carats < >
e.g., all body diagonals: <111> = [111], $[1\bar{1}\bar{1}]$, $[\bar{1}\bar{1}\bar{1}]$, $[1\bar{1}1]$, etc.

all cube edges: <001>
all face diagonals: <011>
all body diagonals: <111>

plane: Miller[1] indices – recall equation of a plane in space

$\frac{x}{a} + \frac{y}{b} + \frac{z}{c} = 1$, where a, b, c are intercepts of the plane with the x, y, z axes, respectively

- let $h = \frac{1}{a}$, $k = \frac{1}{b}$, and $l = \frac{1}{c}$, so that $hx + ky + lz = 1$

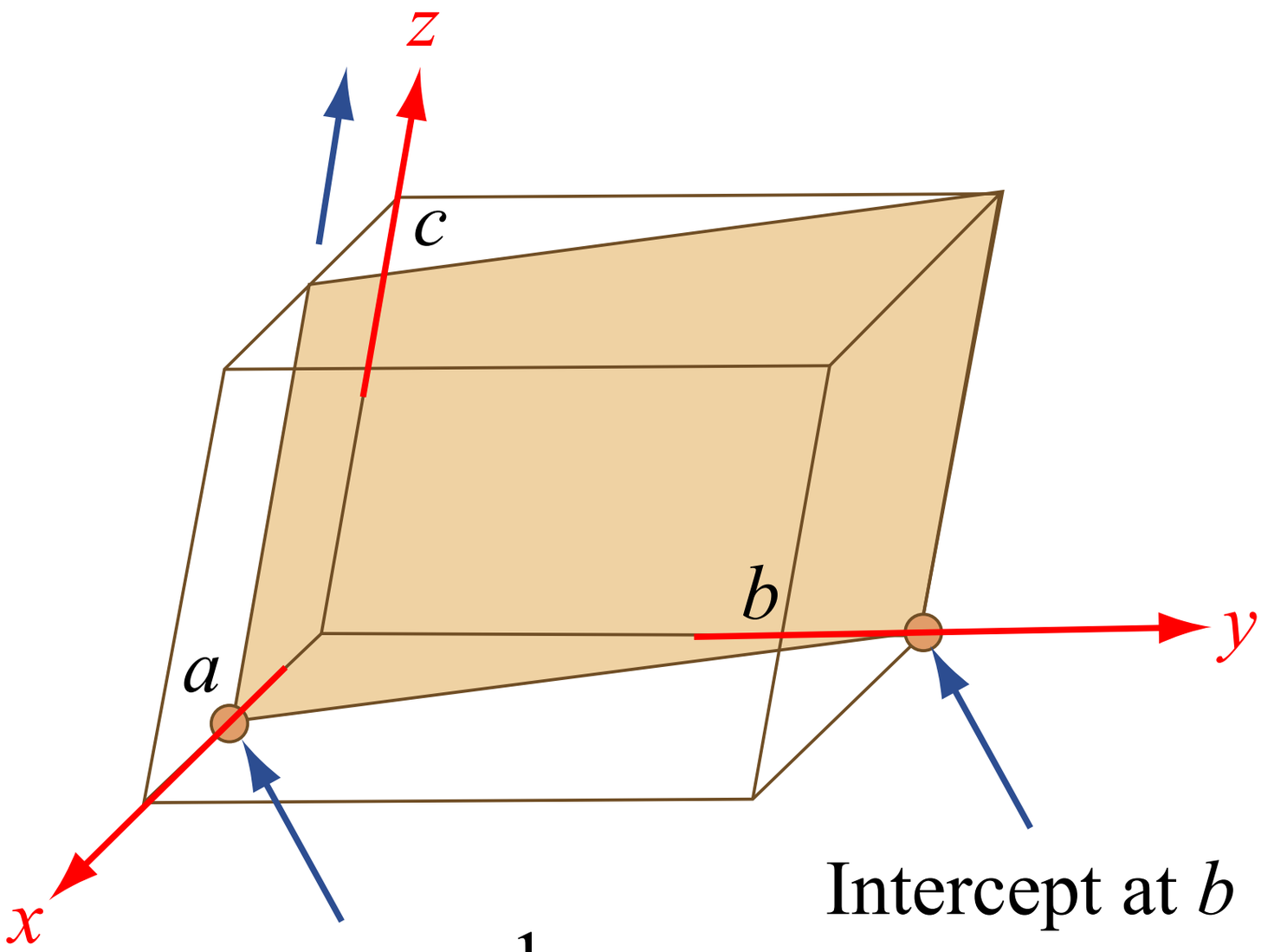
- no commas[2], enclose in parentheses (hkl)

- can denote entire family of planes by braces { }
  e.g., all faces of unit cell: {001} = (001), (00$\bar{1}$), ($\bar{1}$00), (0$\bar{1}$0), etc.

- cool property: (hkl) ⊥ [hkl]

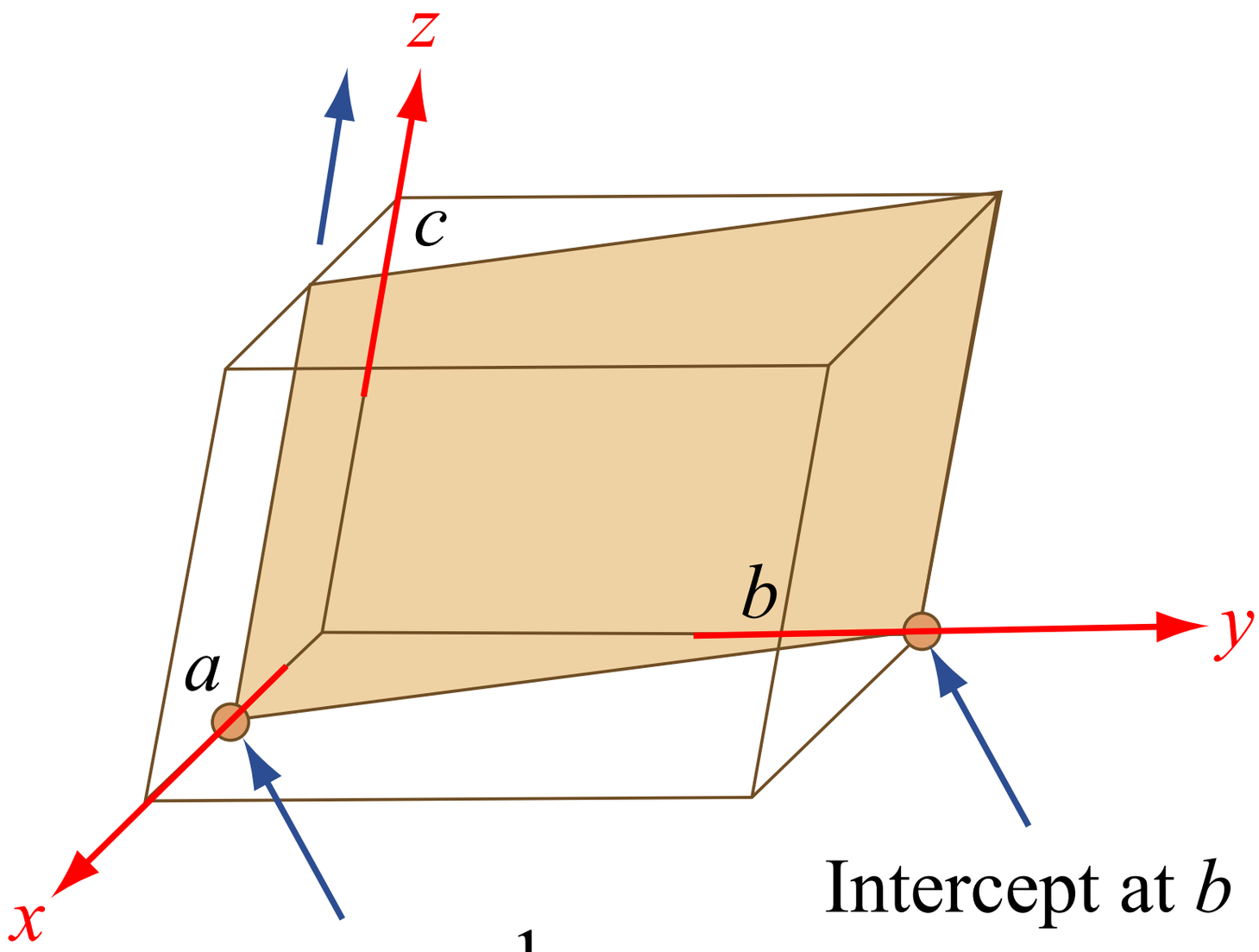
[1] William Hallowes Miller, British mineralogist, 1839
[2] plane must not include the origin

Intercept at ∞



$$\left(\frac{1}{2}, 1, \infty\right)$$

Intercept at ∞



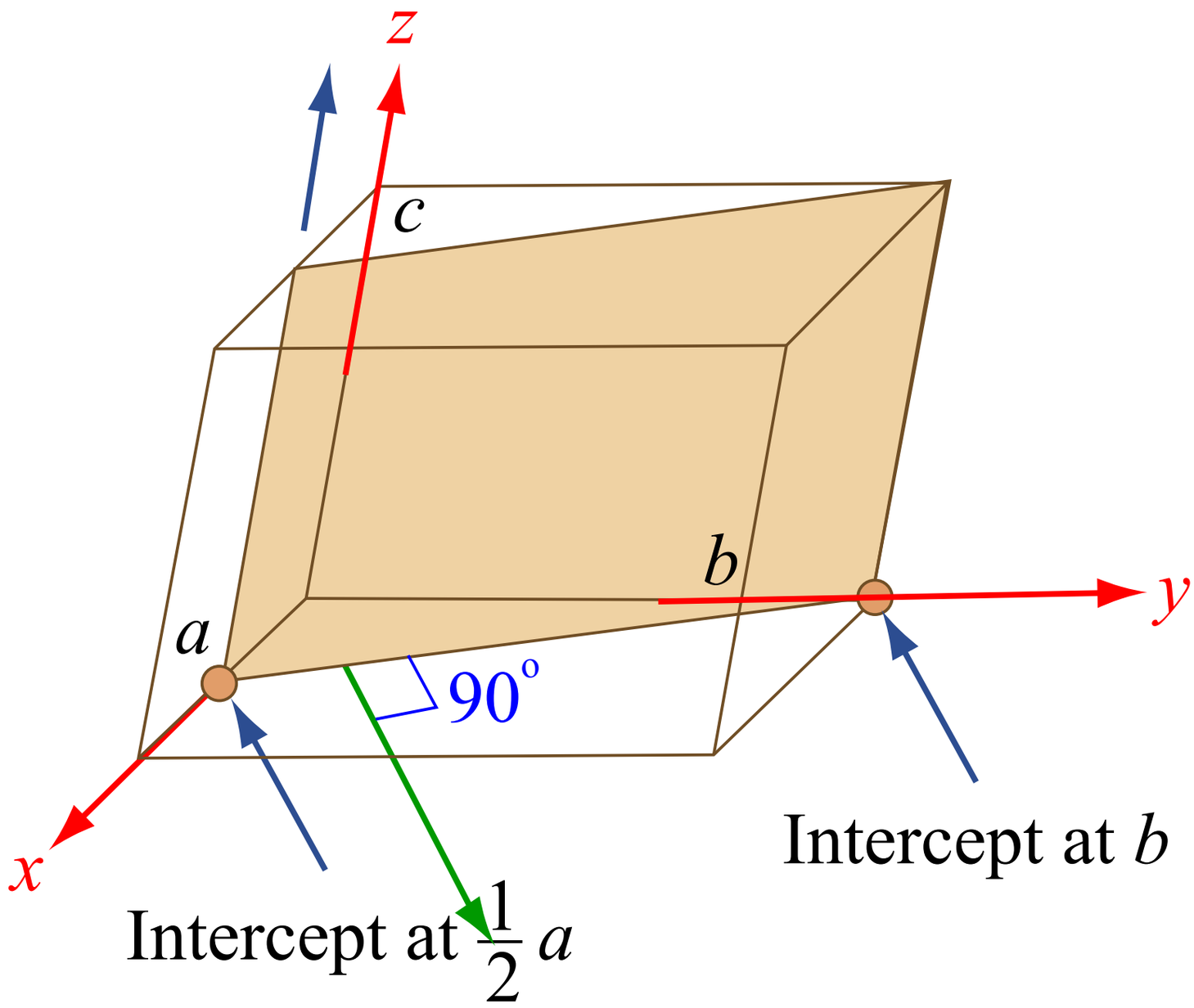
Miller indices (*hkl*):

$$\frac{1}{1/2} \quad \frac{1}{1} \quad \frac{1}{\infty}$$

(210)

Image by MIT OpenCourseWare.

Intercept at ∞



Miller indices (*hkl*):

$$\frac{1}{1/2} \quad \frac{1}{1} \quad \frac{1}{\infty}$$

(210)

Image by MIT OpenCourseWare.

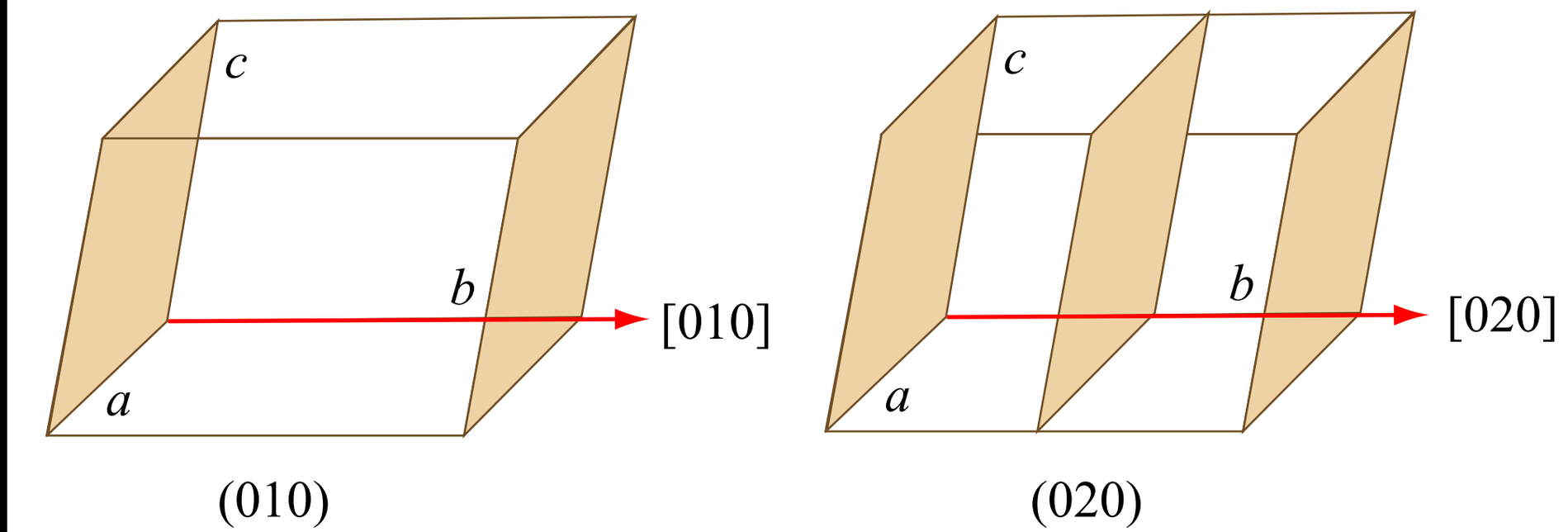


Image by MIT OpenCourseWare.

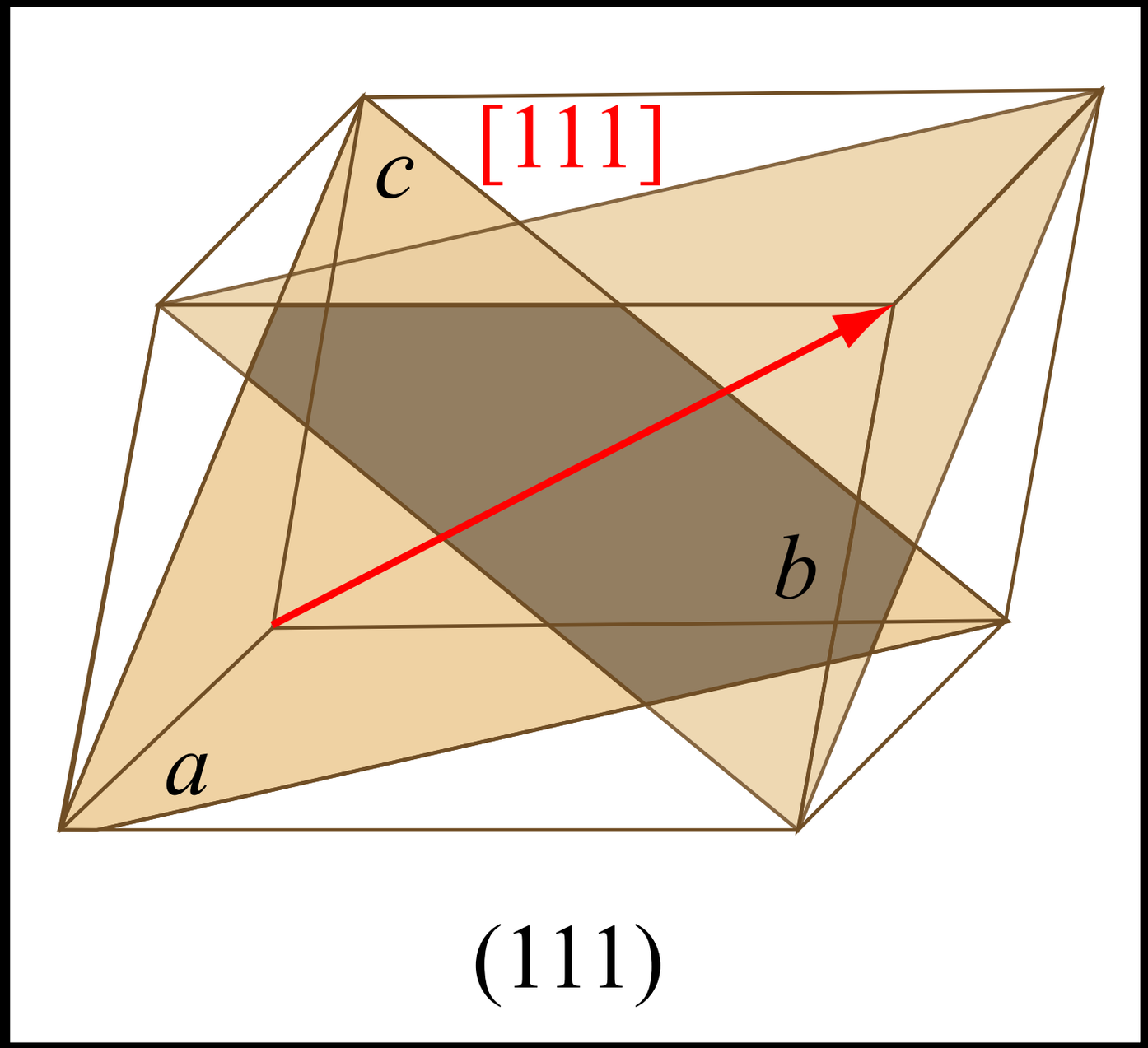
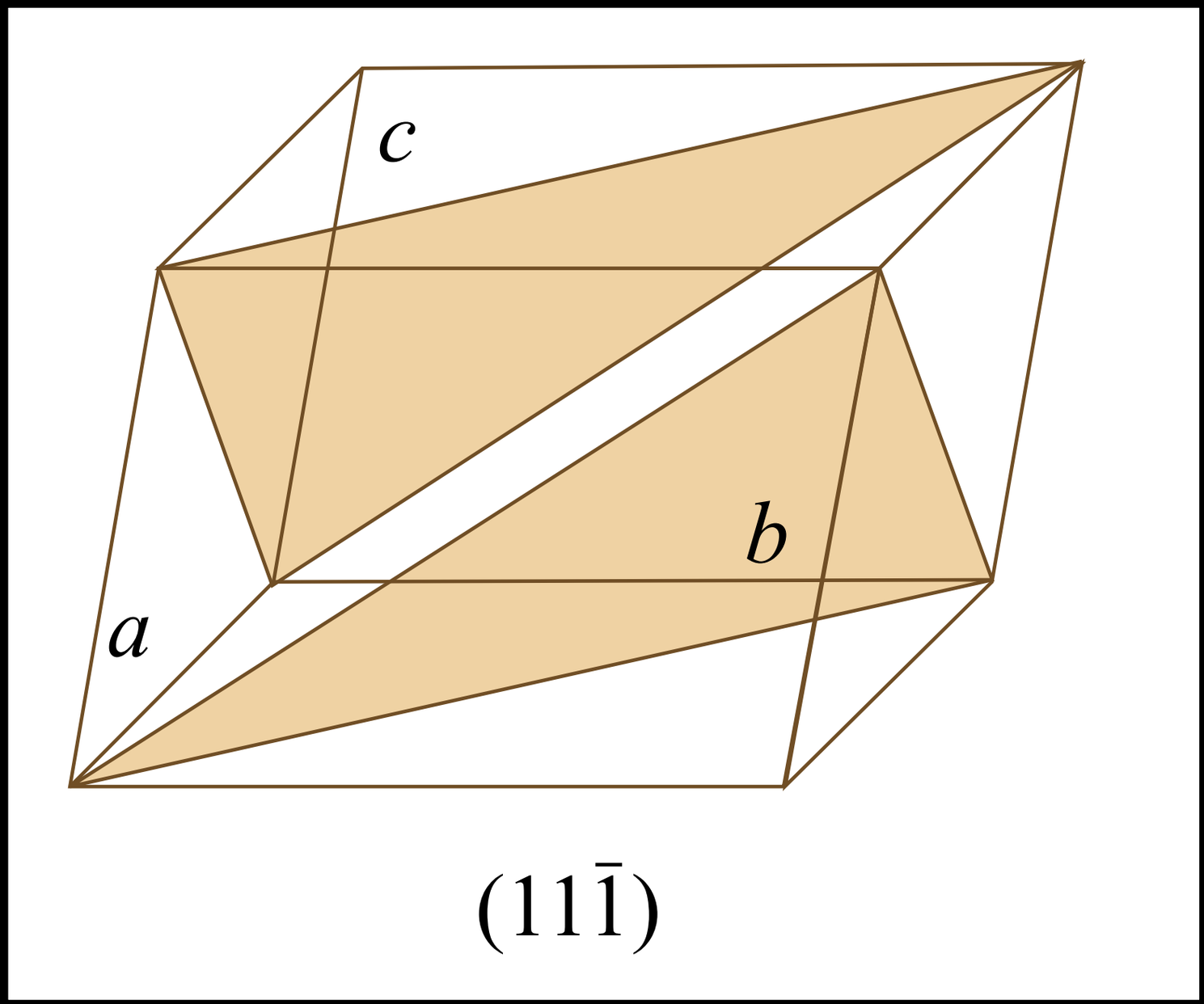
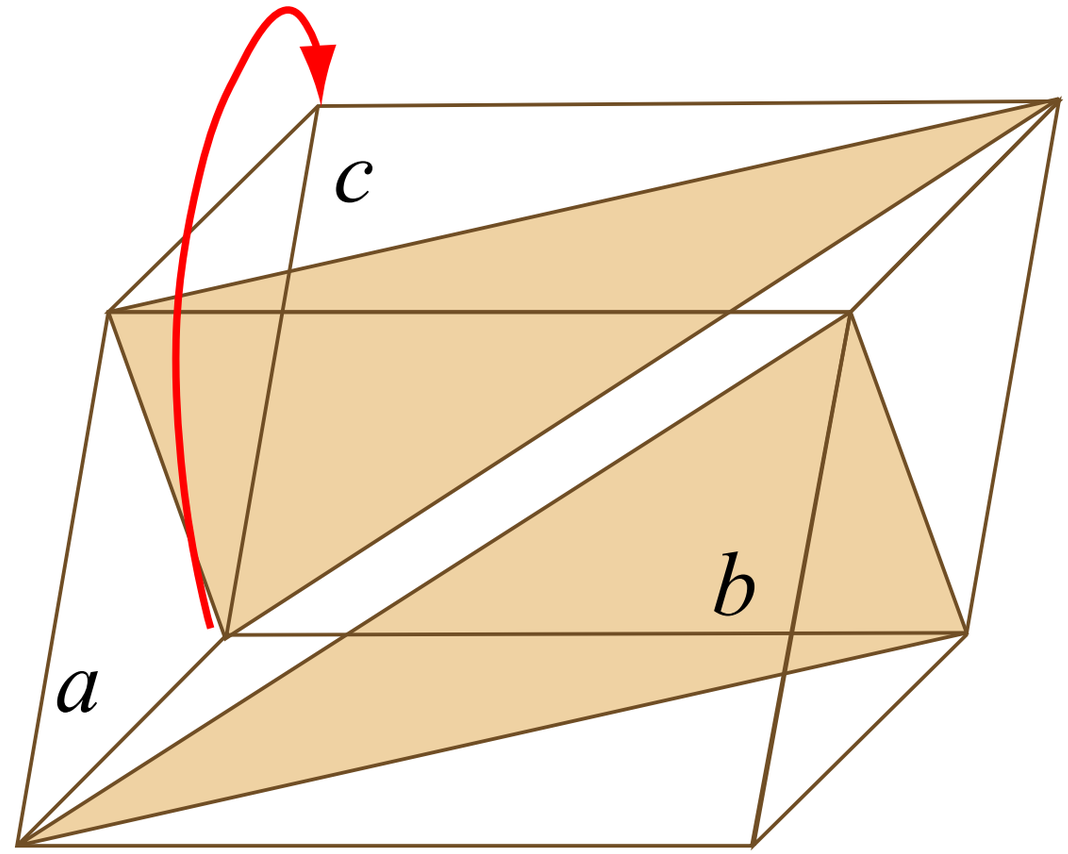


Image by MIT OpenCourseWare.

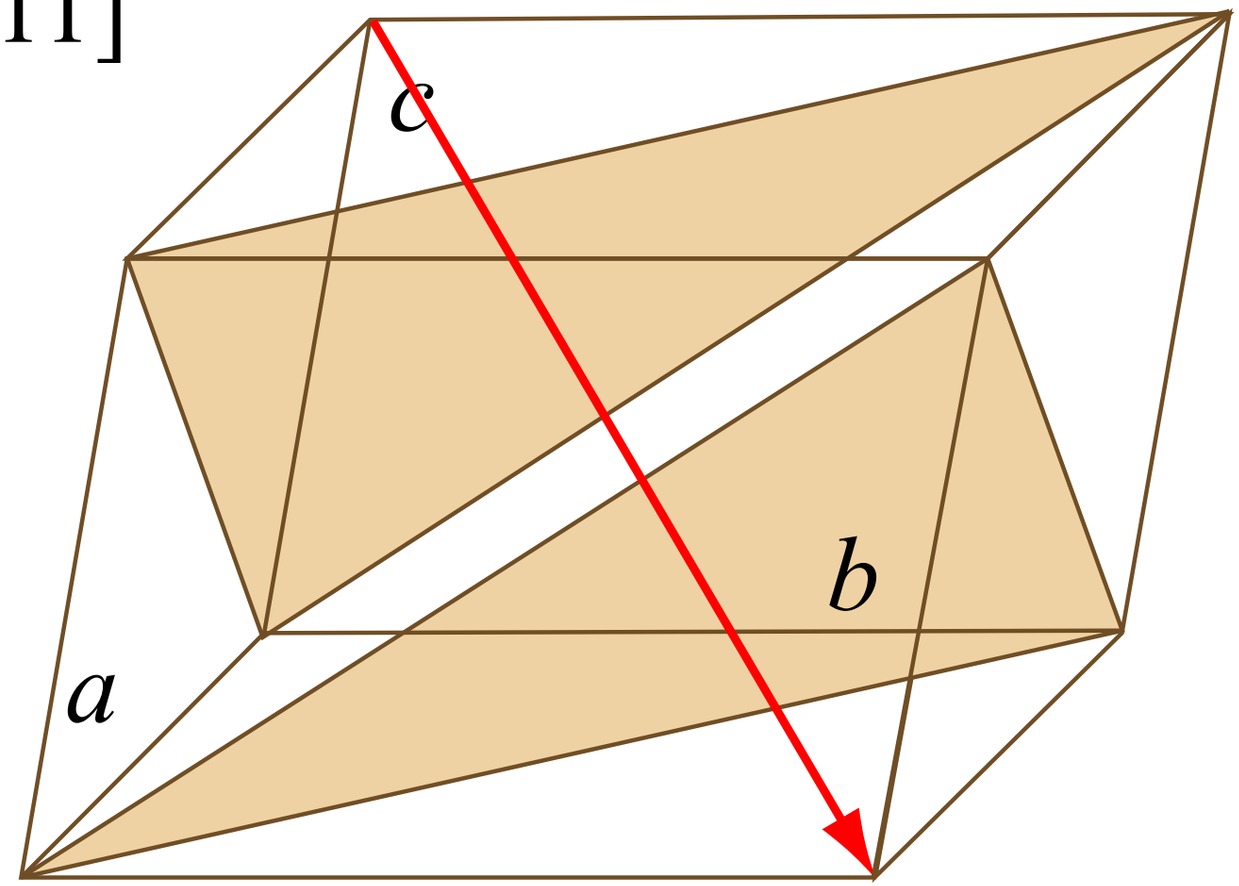


Move the origin out of the plane

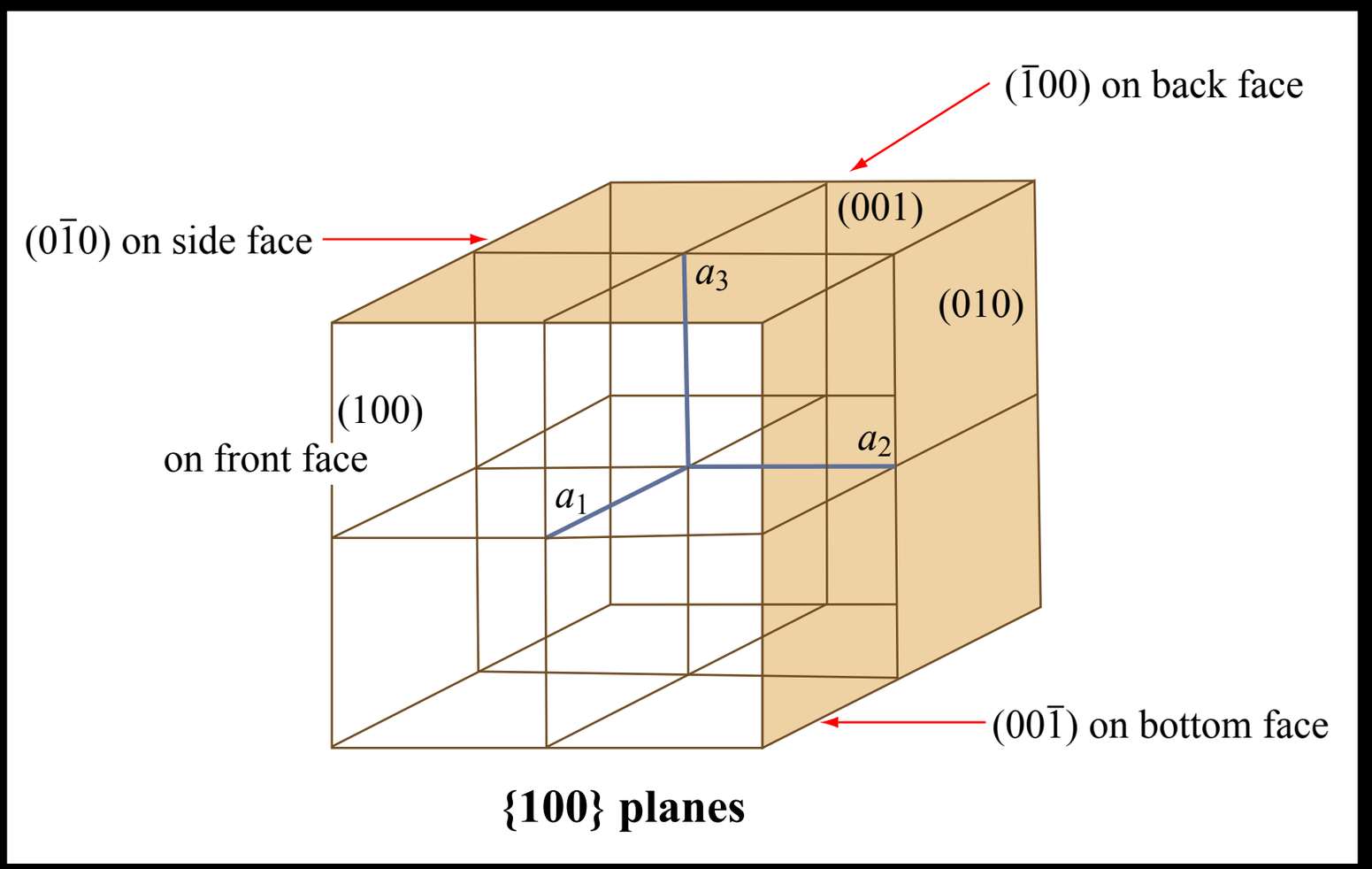


$(11\bar{1})$

$[11\bar{1}]$

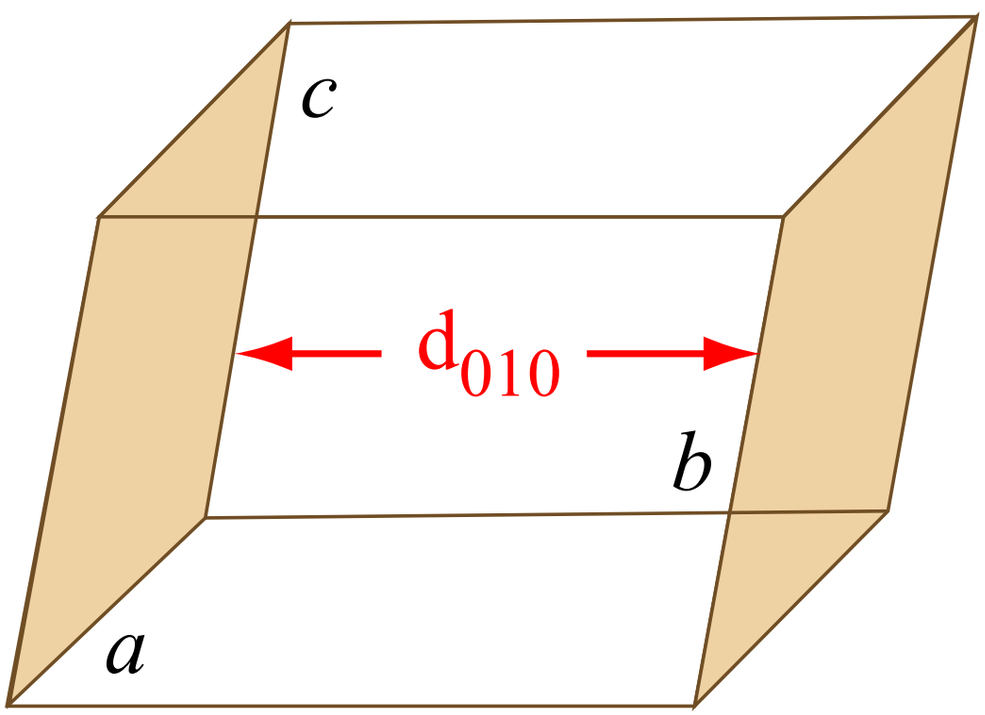


$(11\bar{1})$

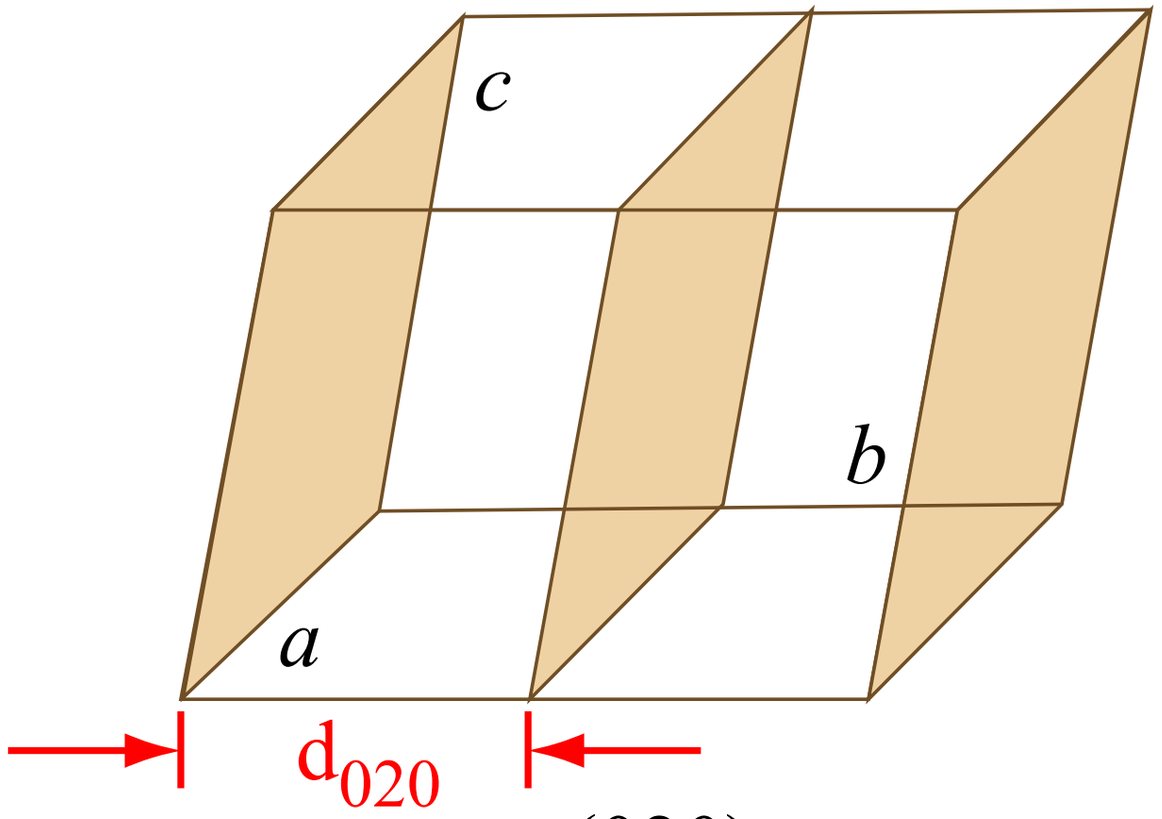


{100} planes

$$a = b = c = \text{"a"} \qquad d_{020} = \frac{a}{(0^2 + 2^2 + 0^2)^{1/2}} = \frac{a}{2}$$

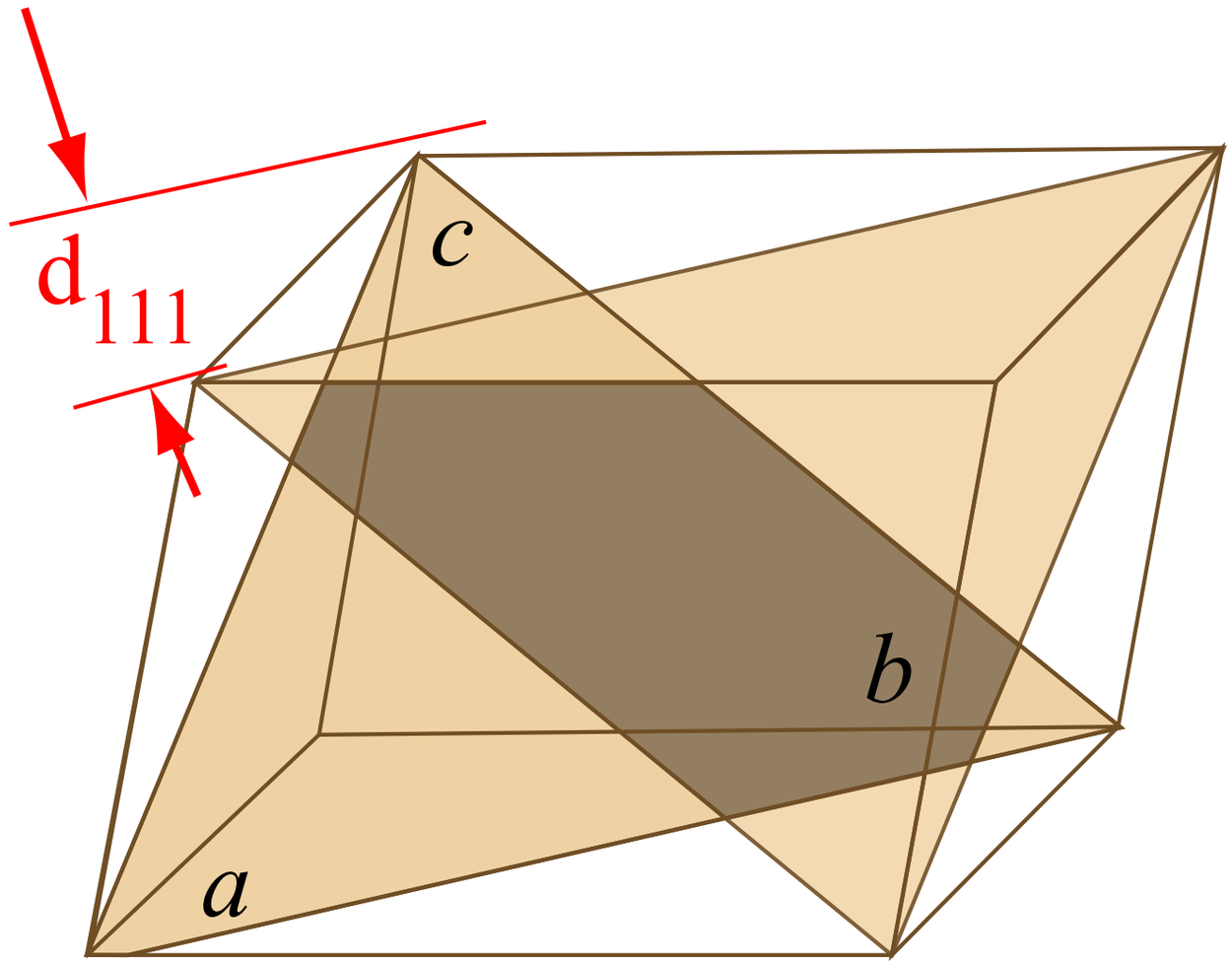


(010)



(020)

$$d_{111} = \frac{a}{(1^2 + 1^2 + 1^2)^{1/2}} = \frac{a}{\sqrt{3}}$$



(111)

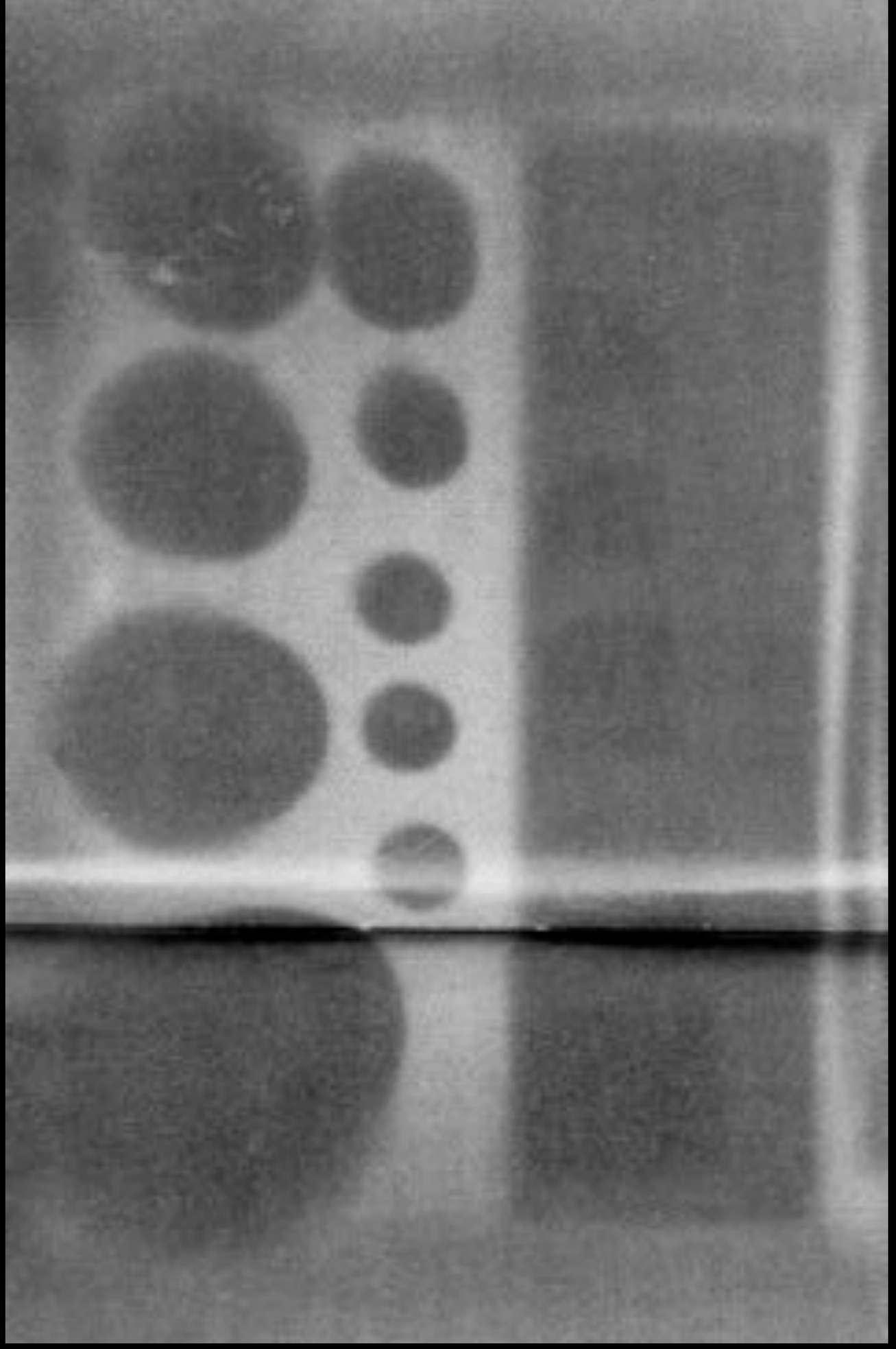
Image by MIT OpenCourseWare.

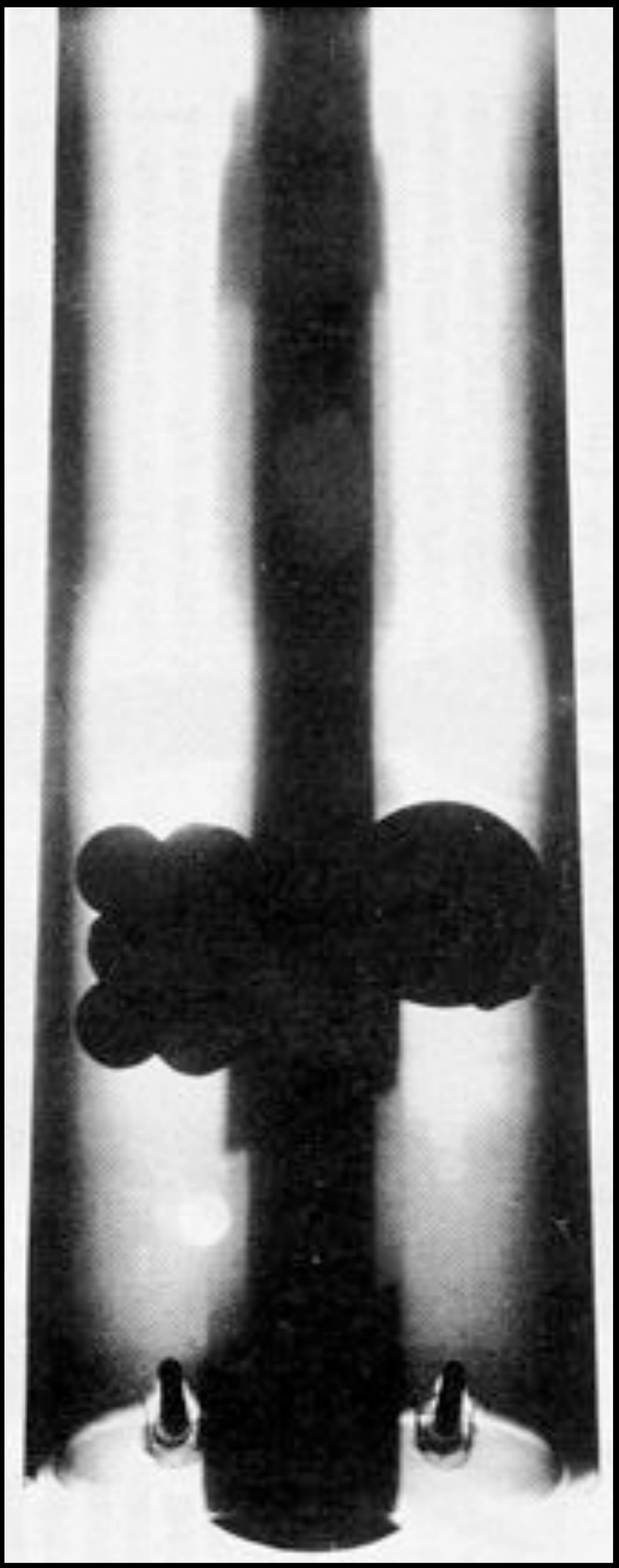
Ionization Energies (eV)

	I	II	III	IV	V	VI	VII
H	**14**	**1**					
He	25	**55**	**4**				
Li	5	76	**123**	**9**			
Be	9	18	154	**218**	**16**		
B	8	25	38	260	**341**	**25**	
C	11	24	48	64	393	**491**	**36**
N	14	30	48	78	98	523	**668**	**49**

$$E_1 = -KZ^2$$

Photos removed due to copyright restrictions. Please see Farmelo, Graham. "The Discovery of X-Rays." *Scientific American* 273 (November 1995): 86-91.





First
Nobel Prize
in Physics
(1901)

3.091SC Introduction to Solid State Chemistry

Fall 2009