

Welcome to 3.091

Lecture 16

October 18, 2004

Crystallographic Notation

position: x,y,z, coordinates, sep^d by commas, no enclosure

O: 0,0,0 **A:** 0,1,1 **B:** 1,0, 1/2

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 1/2 clear fractions  [201]

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

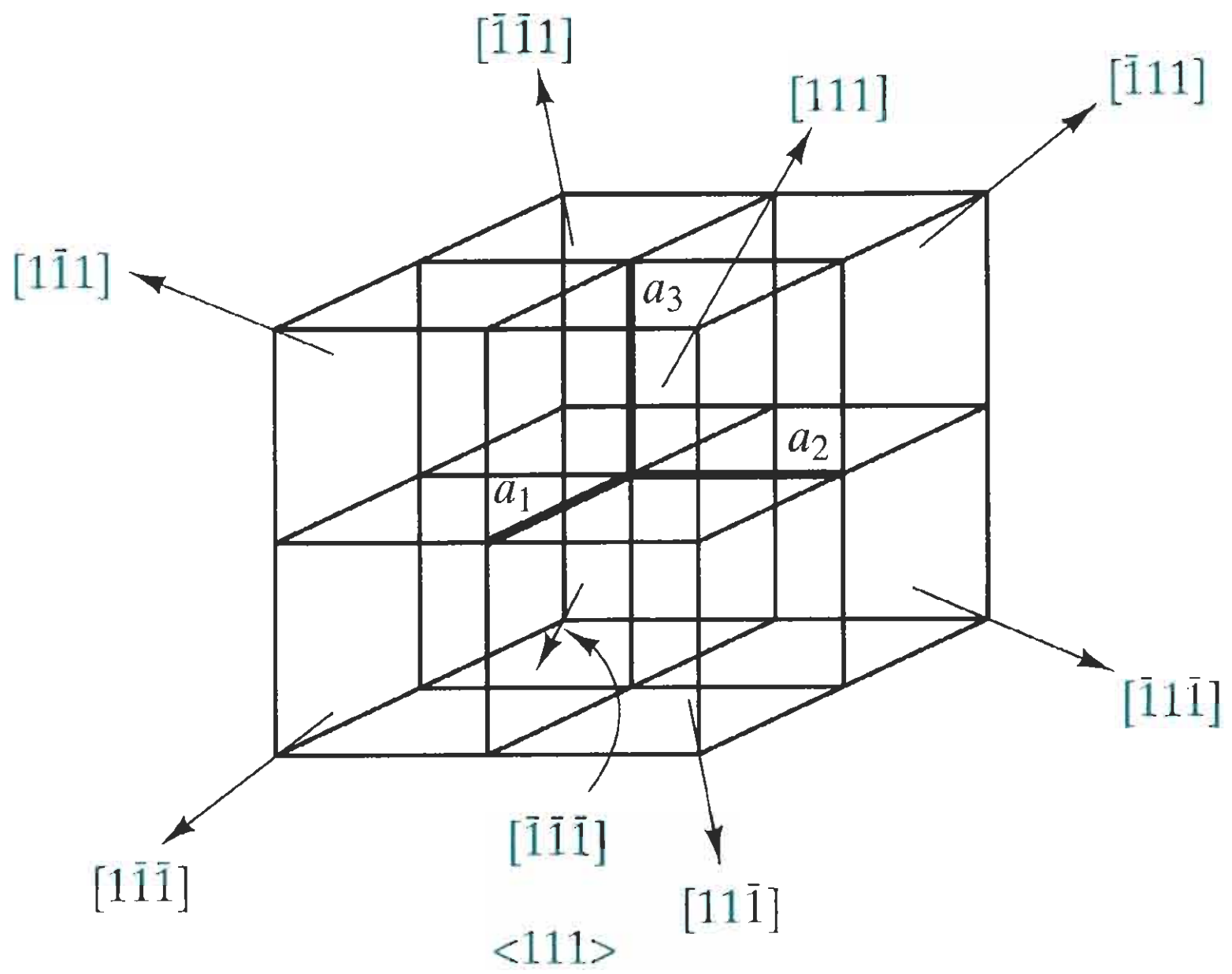
can denote entire family of directions by carats < >

e.g., all body diagonals: <111> = [111], [$\bar{1}\bar{1}\bar{1}$], [$\bar{1}\bar{1}1$], [$1\bar{1}\bar{1}$], etc.

all cube edges: <001>

all face diagonals: <011>

all body diagonals: <111>



plane: Miller¹ indices – recall equation of a plane in space

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

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

- no commas², enclose in parentheses (hkl)

- can denote entire family of planes by braces { }

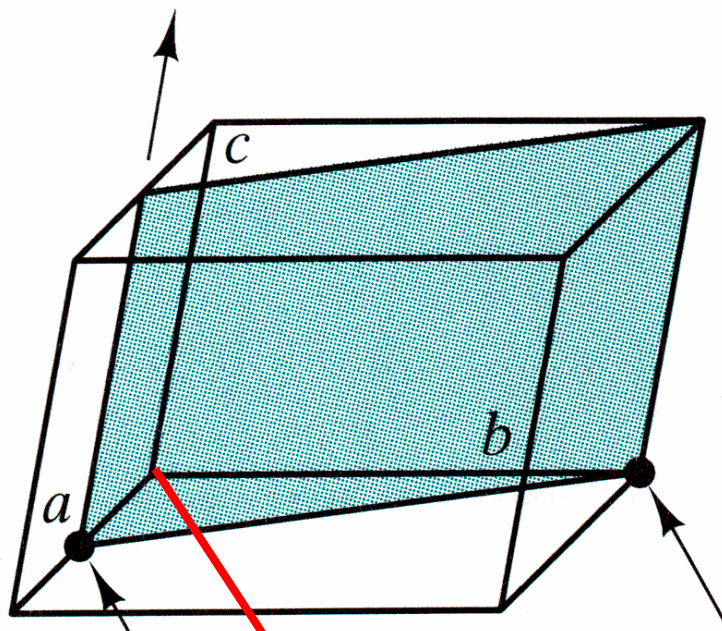
e.g., all faces of unit cell: $\{001\} = (001), (00\bar{1}), (\bar{1}00), (0\bar{1}0), \text{ etc.}$

- cool property: $(hkl) \perp [hkl]$

¹ William Hallows Miller, British mineralogist, 1839

² plane must not include the origin

Intercept at ∞



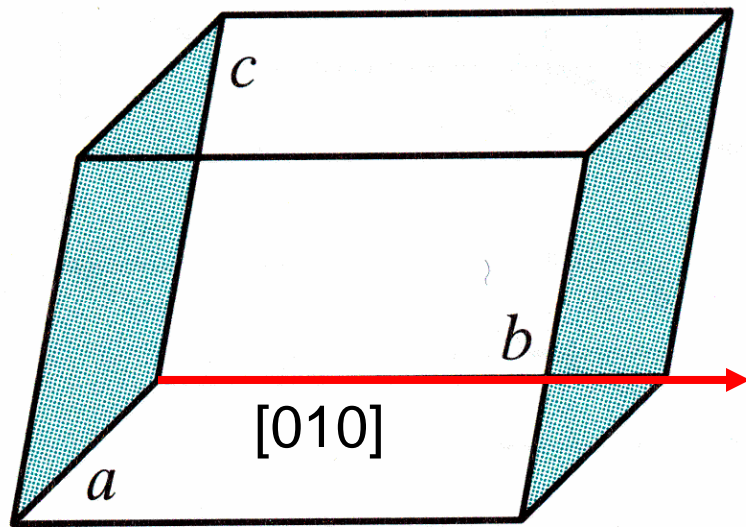
Miller indices (hkl):

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

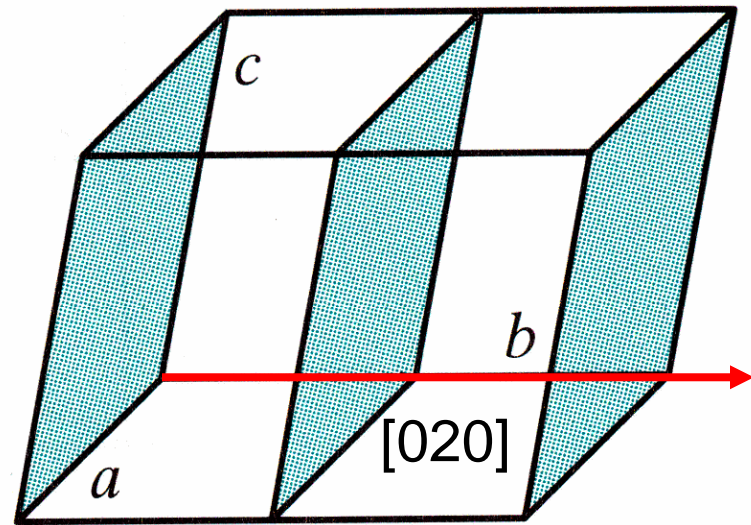
→ (210)

Intercept at $\frac{1}{2} a$

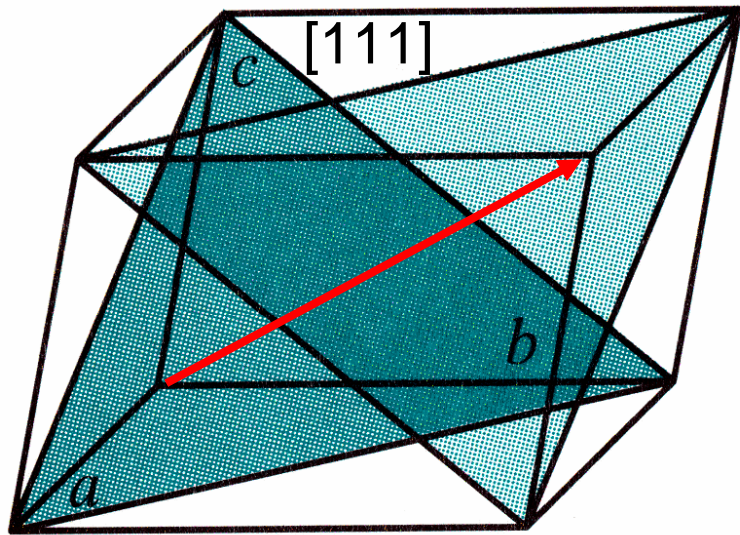
Intercept at b



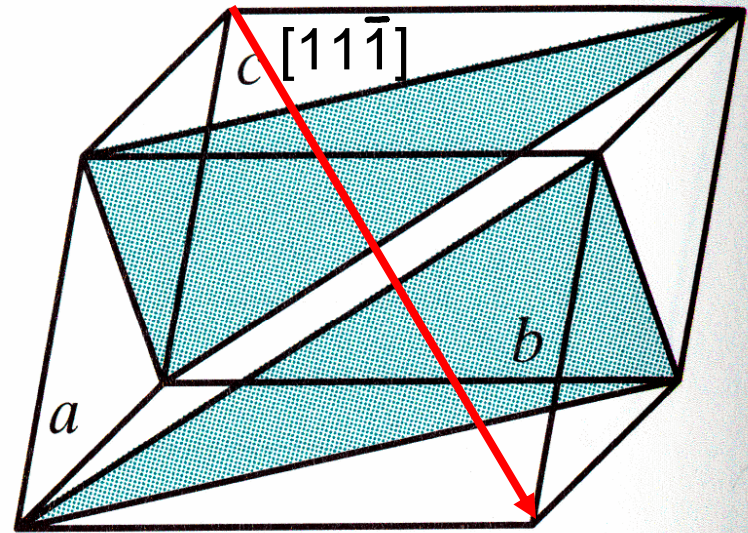
(010)



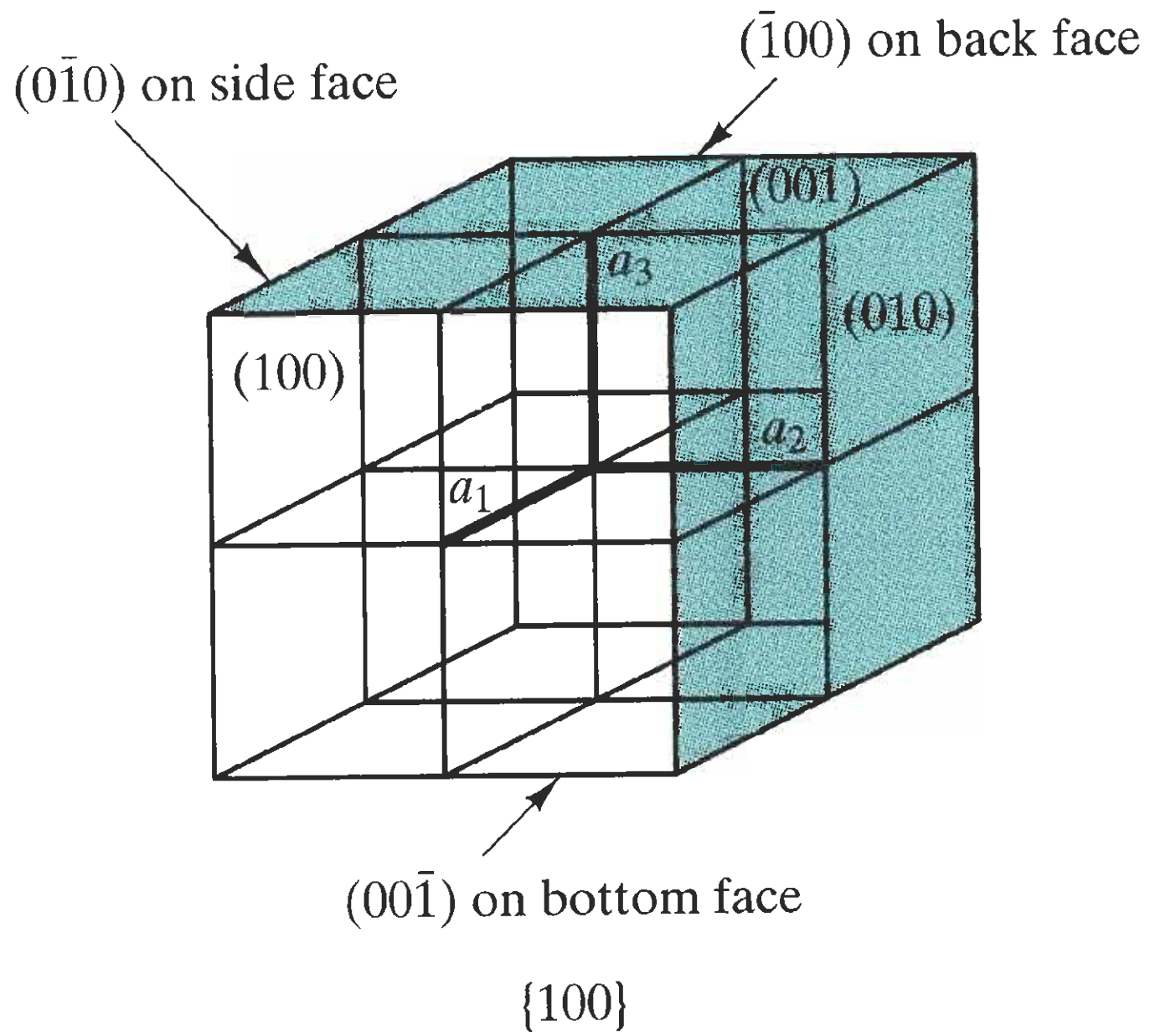
(020)



(111)



(11 $\bar{1}$)



Ionization Energies (eV)

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

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

$$E_n = -KZ^2$$