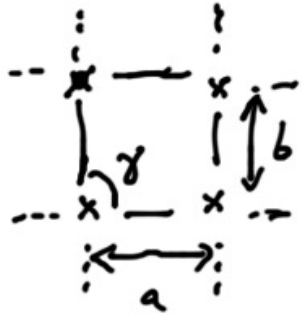
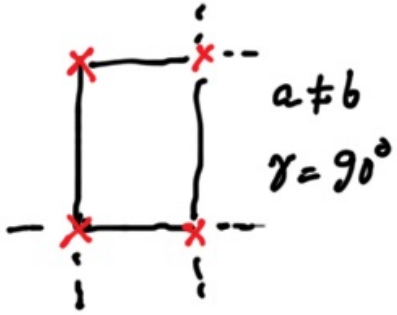
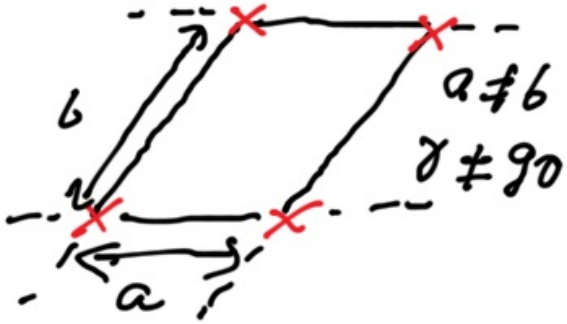
LATTICE PARAMETERS: 2D CASE



a=b
γ=90°



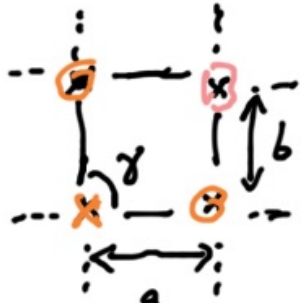
a≠b
γ=90°



a≠b
γ≠90

a, b, γ are lattice parameters

a, b ~ Å ~ 10^{-10} m

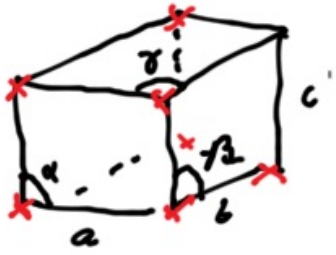


NN = Nearest Neighbours = 4

NNN = Next Nearest Neighbours = 4

Nearest Neighbours (NN)

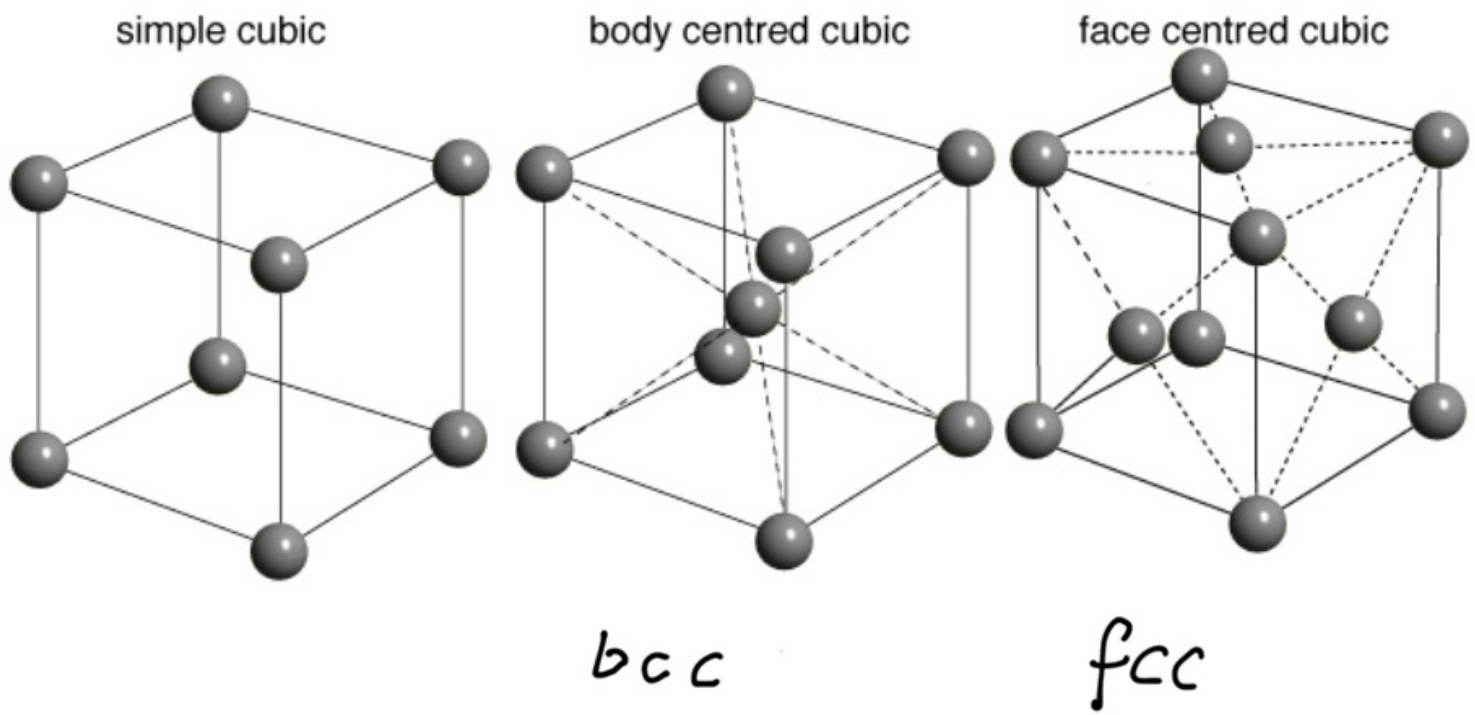
LATTICE PARAMETERS: 3D CASE



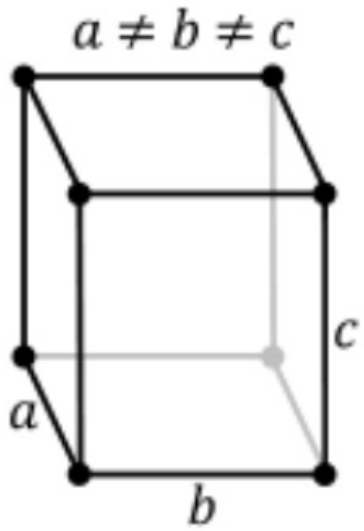
BRAVAIS LATTICIES

STRUCTURES	#		
Cubic	3	$a = = c$;	$\alpha = \beta = \gamma = 90$
Tetragonal	2	$a = b \neq c$;	$\alpha = \beta = \gamma = 90$
Orthorombic	4	$a \neq b \neq c$;	$\alpha = \beta = \gamma = 90$
Hexagonal	1	$a = b \neq c$;	$\alpha = \beta$; $\gamma = 120$
Trigonal	1	$a = b = c$	$90 < \alpha = \beta = \gamma < 120$
Monoclinic	2	$a \neq b \neq c$	$\alpha = \beta = 90 \neq \gamma$
Triclinic	1	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$

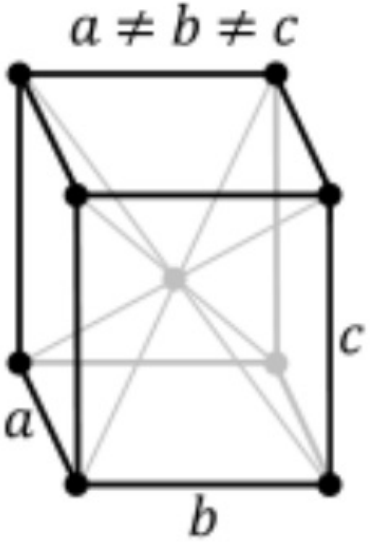
CUBIC CRYSTAL STRUCTURES:



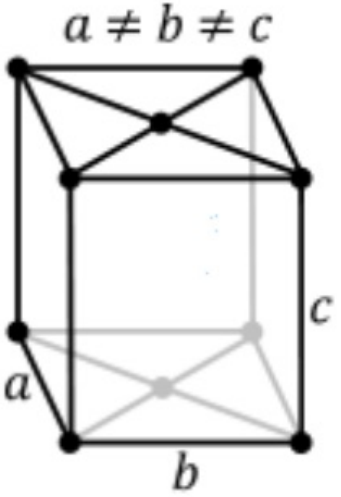
ORTHOROMBIC CRYSTAL STRUCTURES:



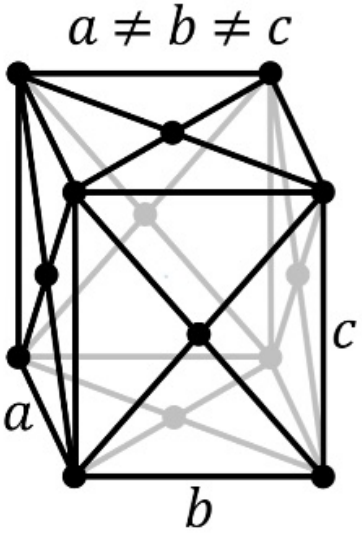
Primitive



Body centered

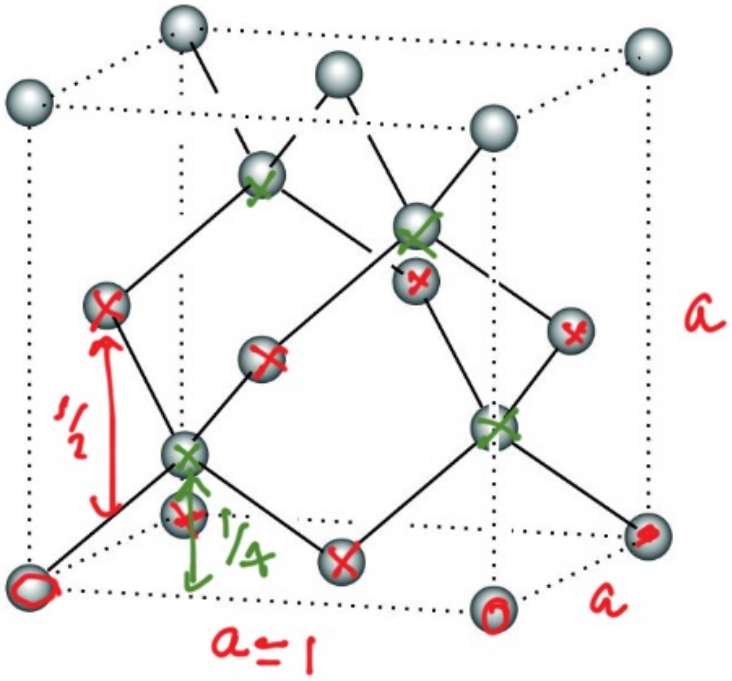


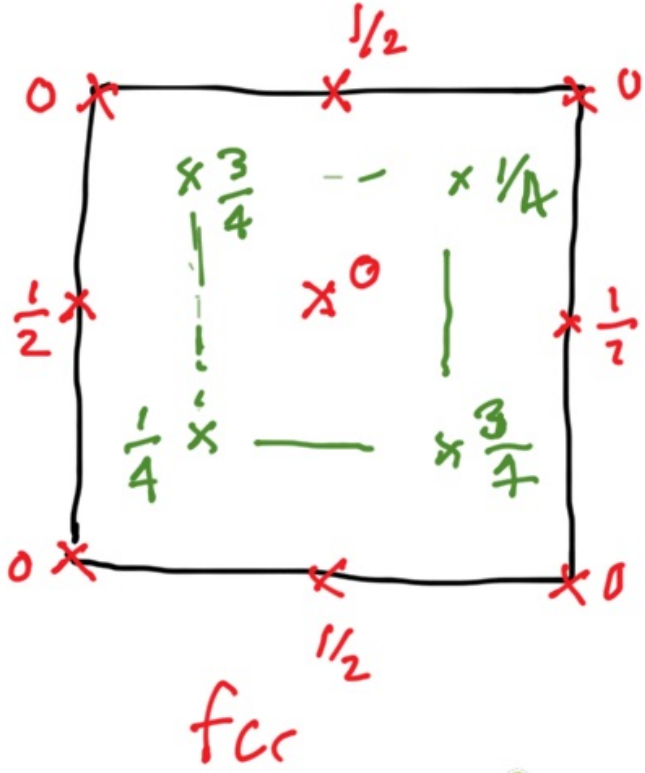
Base centered



Face centered

DIAMOND STRUCTURE:





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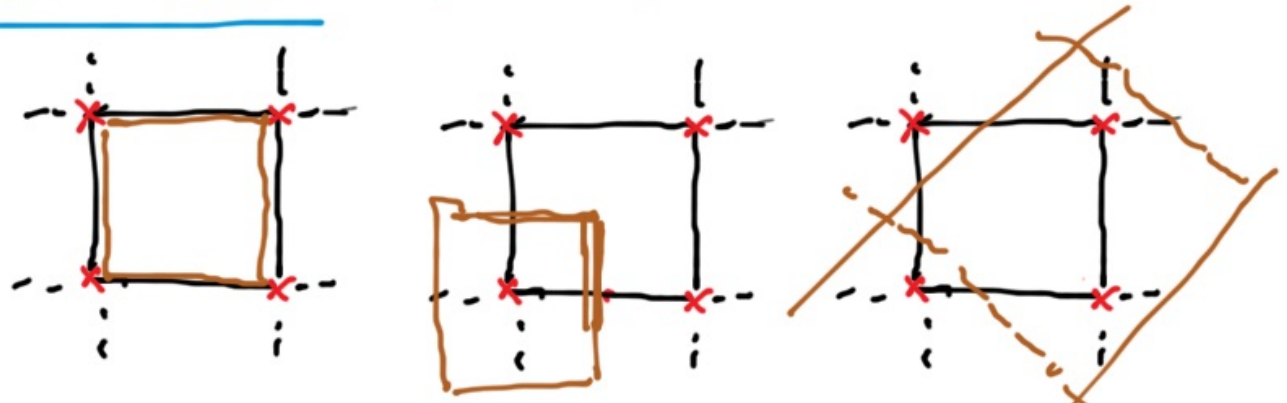
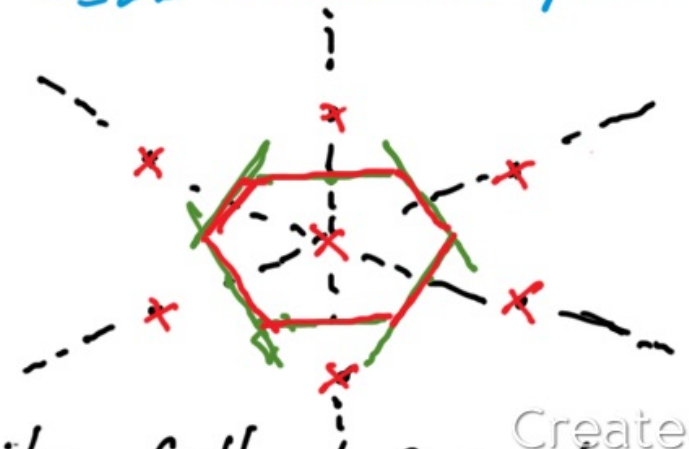
UNIT CELL: A REPEATED STRUCTURAL UNIT



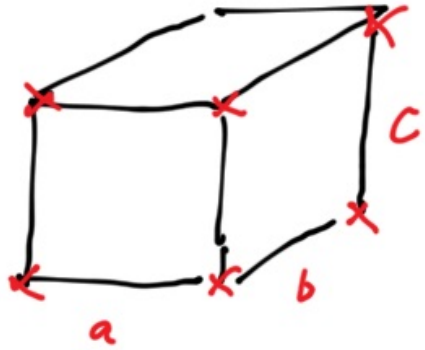
A UNIT CELL IS NOT UNIQUELY DEFINED

PRIMITIVE CELL = smallest possible unit cell



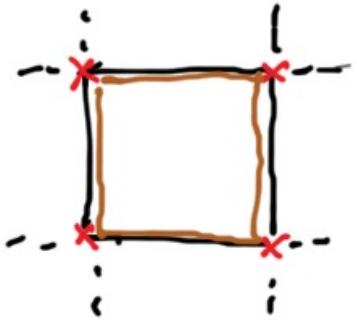
Wigner-Seitz Cell = Primitive cell

VOLUME OF UNIT & PRIMITIVE CELL:



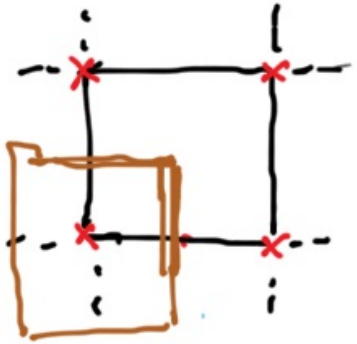
$V(\text{unit cell}) = a \times b \times c$

NUMBER OF ATOMS (LATTICE POINTS) PER V(UNITCELL)



$4 \times \frac{1}{4} \frac{\text{Atoms}}{V(\text{unit cell})}$

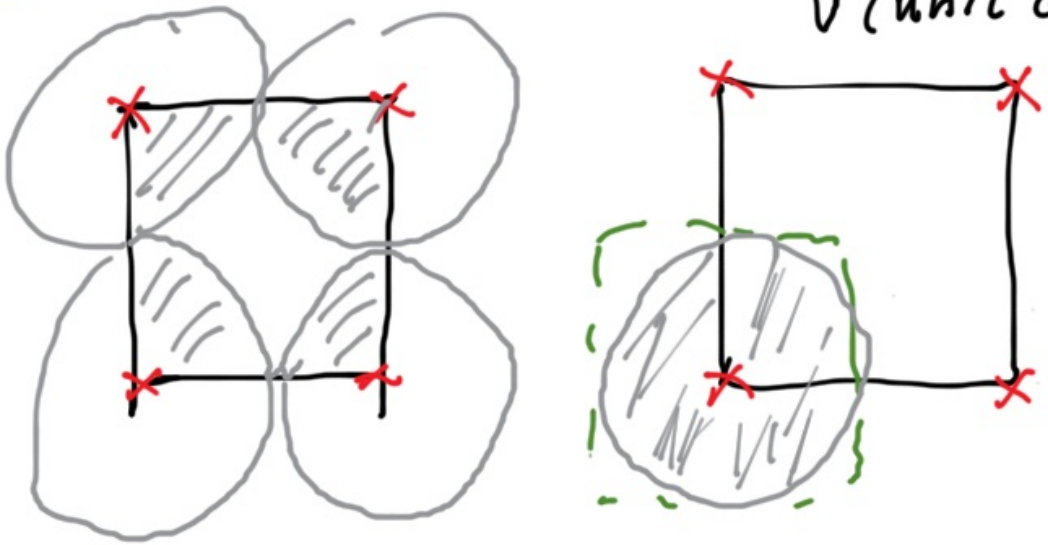
Each corner atom is shared by 4 unit cells.



$\frac{1 \text{ atom}}{V(\text{unit cell})}$

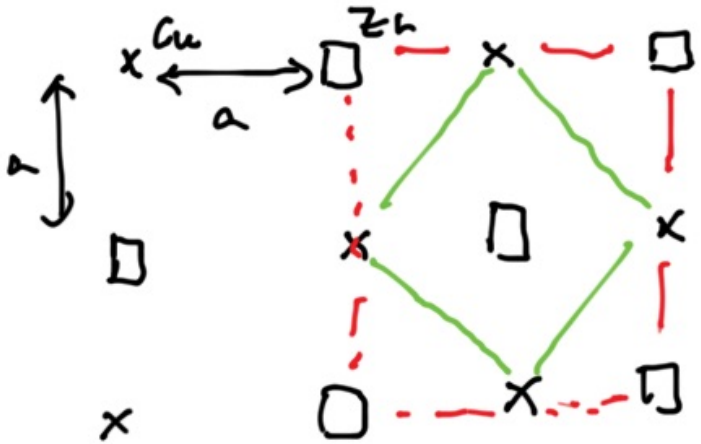
$\text{Mass density} = \frac{\sum \text{atomic mass}}{V(\text{unit cell})}$

PACKING RATIO = $\frac{N_{atoms} \cdot V_{atom}}{V(\text{unit cell})}$



Gray shaded area is the V_{atom} volume.

EXAMPLE: BRASS (MESSING) IN 2D



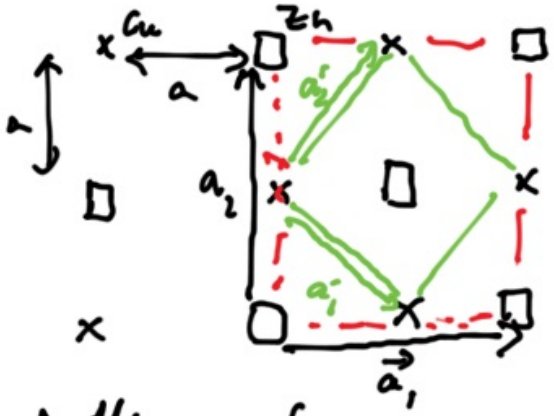
NN distance $= \sqrt{2}\,a$

NNN distance $= 2a$

$$\frac{\#\ \text{atoms}}{V(\text{unit cell})} = \frac{1\,Zn + 4\cdot\frac{1}{4}\,Cu}{\sqrt{2}a \cdot \sqrt{2}a} = \frac{1\,Zn + 1\,Cu}{2a^2}$$

$$\frac{\#\ \text{atoms}}{V(\text{unit cell})} = \frac{1 + 4\cdot\frac{1}{4}\,Zn + 4\cdot\frac{1}{2}\,Cu}{4a^2} = \frac{2}{4}\,\frac{1\,Zn + 1\,Cu}{a^2}$$

LATTICE VECTORS:



Lattice vectors are not uniquely defined

$a_1 = \{1, 0\}$ $a_2 = \{0, 1\}$

$a_1' = \{1, 0\}$ $a_2' = \{0, 1\}$

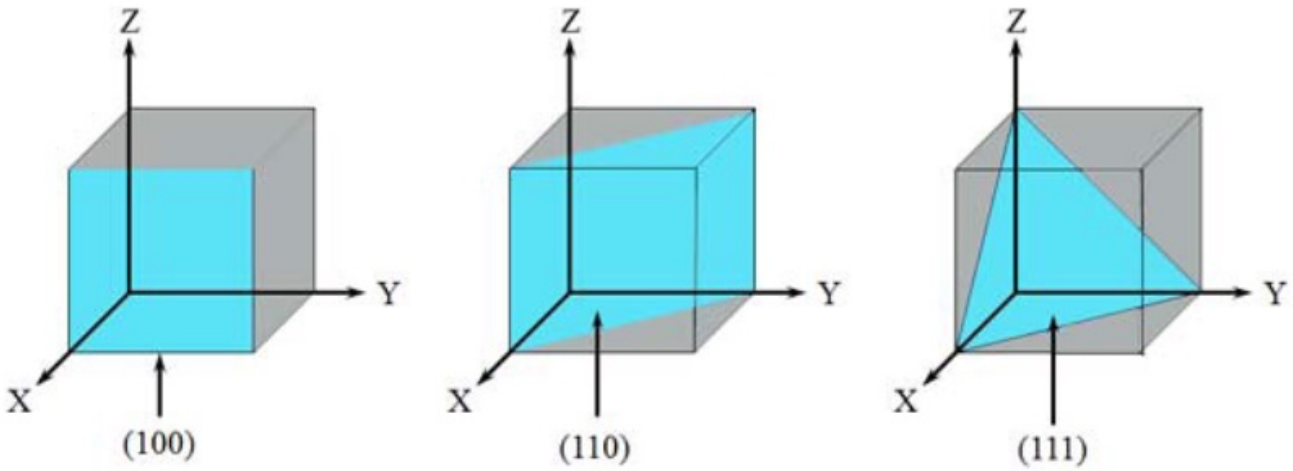
Basis $= \{ \vec{r}_{Cu}, \vec{r}_{Zn} \}$

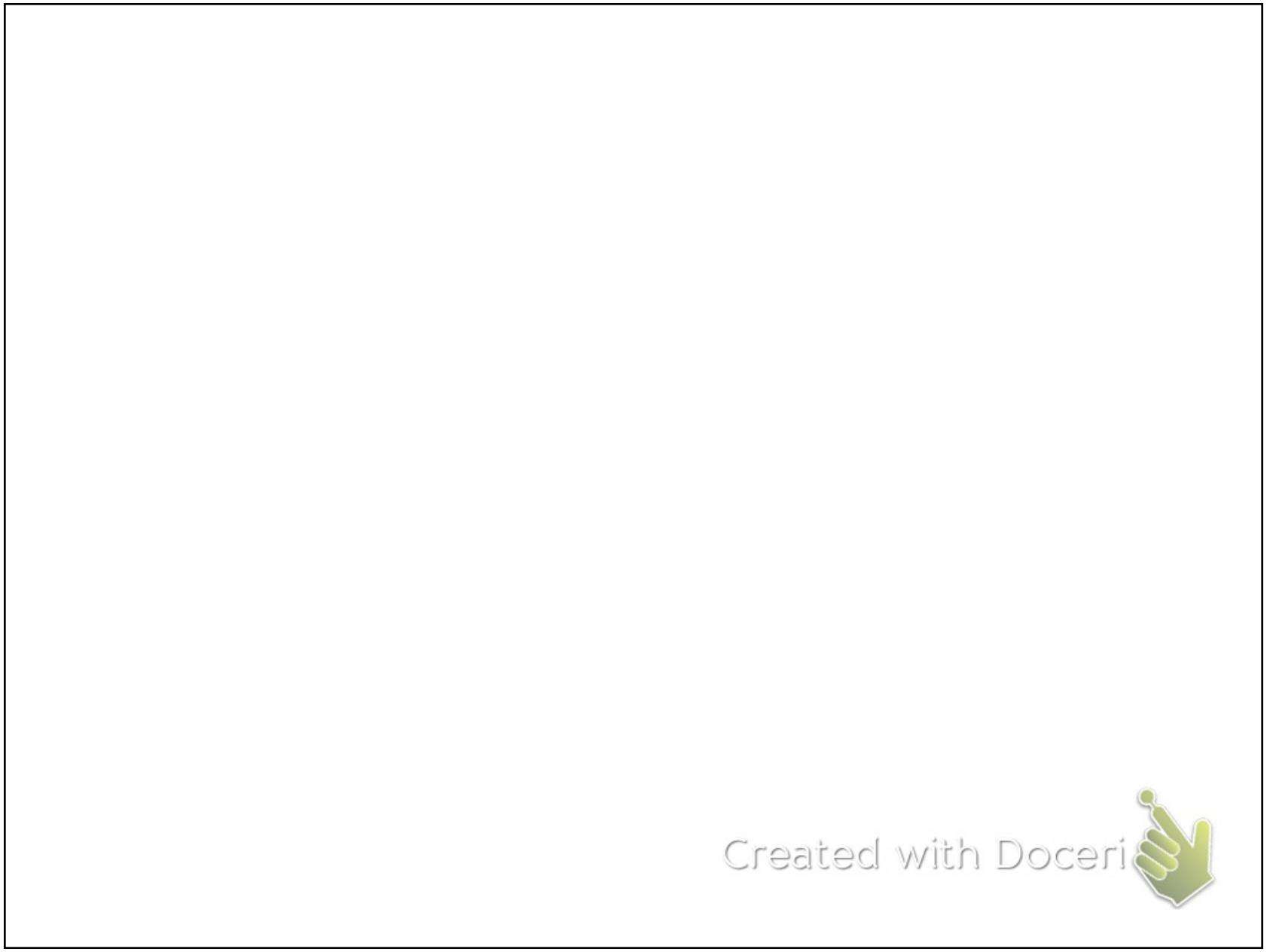
$$\text{Lattice} = \text{Basis} + u_1 \cdot \vec{a}_1 + u_2 \vec{a}_2$$

$$= \text{Basis} + u_1' \cdot \vec{a}_1' + u_2' \vec{a}_2'$$

Where u_1, u_2, u_1', u_2' are integers.

CRYSTAL PLANES:

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