IN CLASS # 1

1. The atomic radii of body-centered cubic (BCC) Fe and face-centered cubic (FCC) Fe are 1.241 Å and 1.269 Å. Calculate the lattice parameters of both BCC and FCC Fe.
2. Calculate the interplanar spacing between the (111) planes of gold (Au) whose lattice parameter is 4.0786 Å. If Cr radiation (λ=2.291 Å) is used to determine this Au sample, what will be the diffraction angle (2θ)?
3. Atomic radius of copper (Cu) is 0.128 nm. The crystal structure of Cu is face-centered cubic (FCC). Its atomic mas is 63.5 g/mol. Calculate the theoretical density of Cu. (<u>For comparison:</u> experimental real density of Cu is 8.94 g/cm^3).
4. Draw the following directions and planes in a unit cell.
   $[1\bar{1}0]$, [111], [110], [120]
   $(0\bar{1}1)$, (001), (101), $(0\bar{1}2)$

SOLUTIONS OF IN CLASS # 1

1) Lattice parameter for cubic crystal structures is designated as "a".

<u>For BCC Fe</u>: the relation between atomic radius (R) and lattice parameter (a)

$$a = \frac{4R}{\sqrt{3}} = \frac{4.(1,241)}{\sqrt{3}} = 2,87 A^\circ$$

$$1 Å = 10^{-1} nm \qquad a = 0,287 \, nm$$

<u>For FCC Fe:</u> $a = \dfrac{4R}{\sqrt{2}} = \dfrac{4.(1,269)}{\sqrt{2}}$

$$a = 3,59 Å = 0,359 \, nm$$

2) Au (gold) → FCC

For cubic crystal structures,

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

a → lattice parameter (unit cell edge length)

d_{hkl} → interplanar spacing

$d_{hkl} \rightarrow d_{111}$

$$d_{111} = \frac{4.0786\ \text{Å}}{\sqrt{1^2+1^2+1^2}} = \frac{4.0786}{\sqrt{3}}$$

$$d_{111} = 2{,}355\ \text{Å} = 0{,}2355\ \text{nm}$$

Bragg's Law : $\underbrace{\lambda}_{\text{wavelength of X-rays}} = 2\underbrace{d}_{\text{interplanar spacing}} . \sin \underbrace{\theta}_{\text{angle of diffracted beam}}$

$$d_{hkl} = \frac{\lambda}{2d \sin\theta} \rightarrow d_{111} = \frac{2{,}291\ \text{A}^\circ}{2 . \sin\theta}$$

$$2{,}355\ \text{Å} = \frac{2{,}291\ \text{Å}}{2 . \sin\theta} \qquad \sin\theta = \frac{2{,}291}{2 . 2{,}355}$$

$$\sin\theta = 0{,}4864 \Rightarrow \theta = 29{,}1^\circ$$

$$\underbrace{2\theta}_{\text{diffraction angle}} = 58{,}2^\circ$$

3) Theoretical density of Cu can be calculated with the below equation:

$$\rho = \frac{n . A_{Cu}}{V_C . N_A}$$

n: number of atoms associated with each unit cell.

A: atomic weight $\quad V_C$: volume of unit cell

N_A: Avagadro's number ($6{,}022 \times 10^{23}$ atoms/mol)

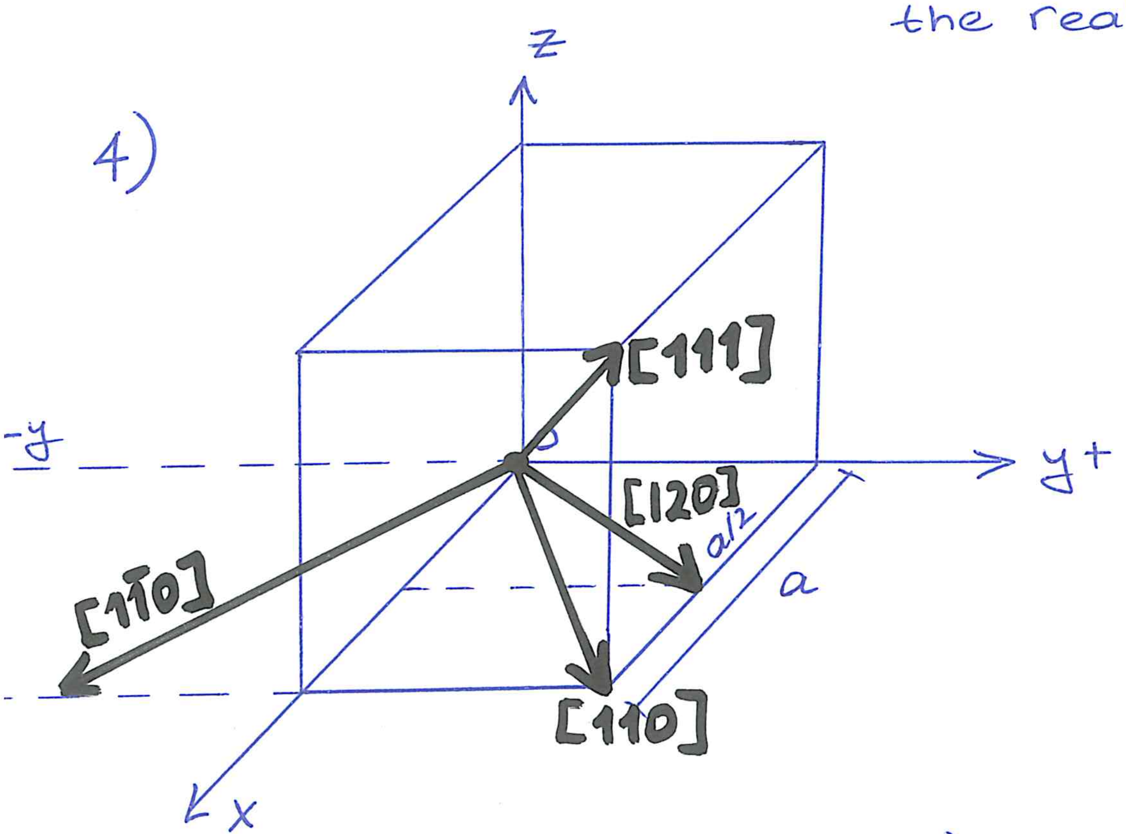
Cu → FCC → 4 atoms per unit cell

$$V_c = a^3 = \left(\frac{4R}{\sqrt{2}}\right)^3 = 16 . R^3 . \sqrt{2}$$

$$\rho = \frac{(\underset{\text{atoms}}{4})(63{,}5\ g/mol)}{16\sqrt{2}\,(1{,}28 . 10^{-8}\ cm)^3\left[6{,}023 . 10^{23}\ \frac{atoms}{mol}\right]}$$

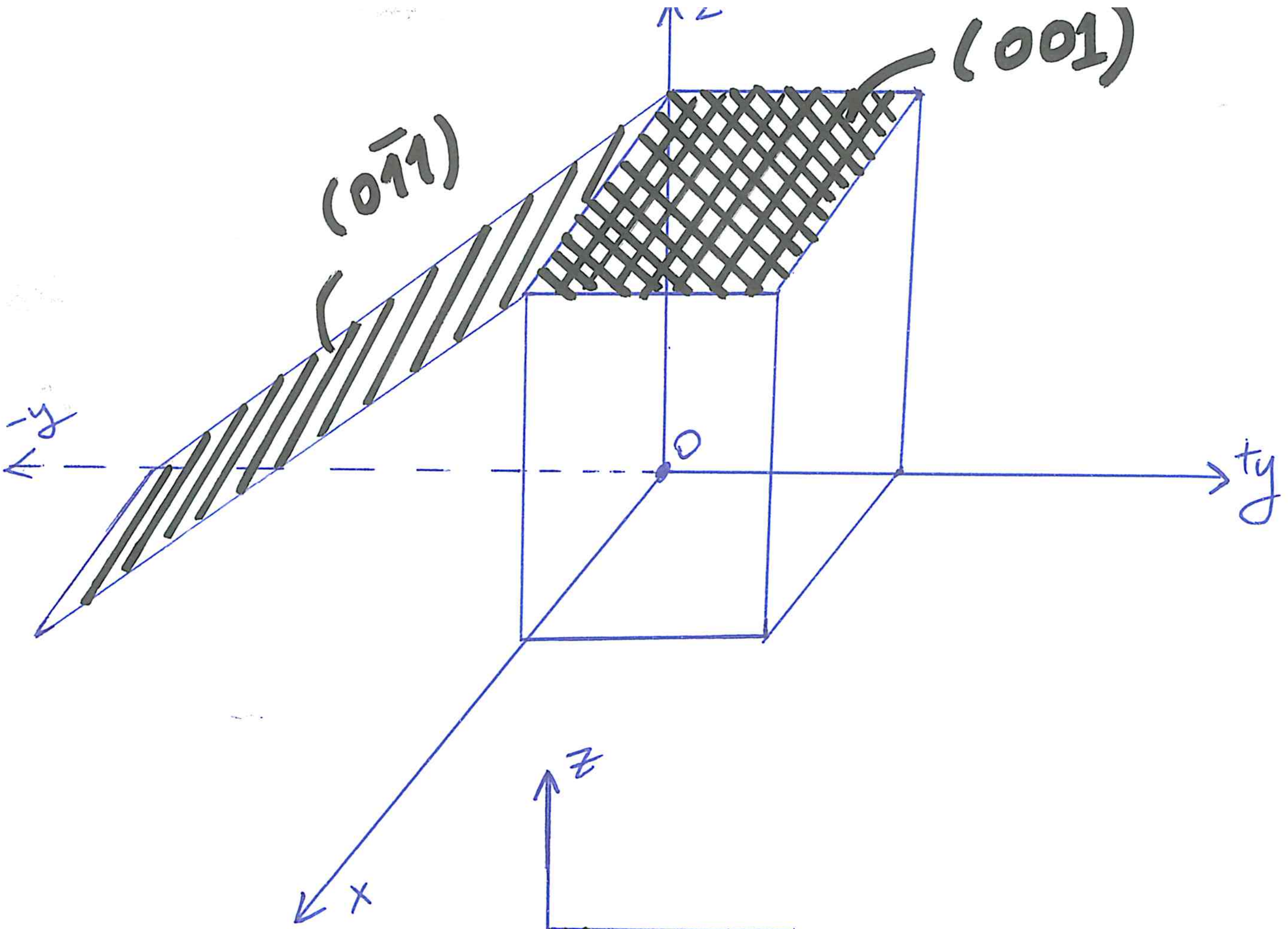
$\rho = 8{,}89\ g/cm^3$ Theoretical density is found close to the real density.

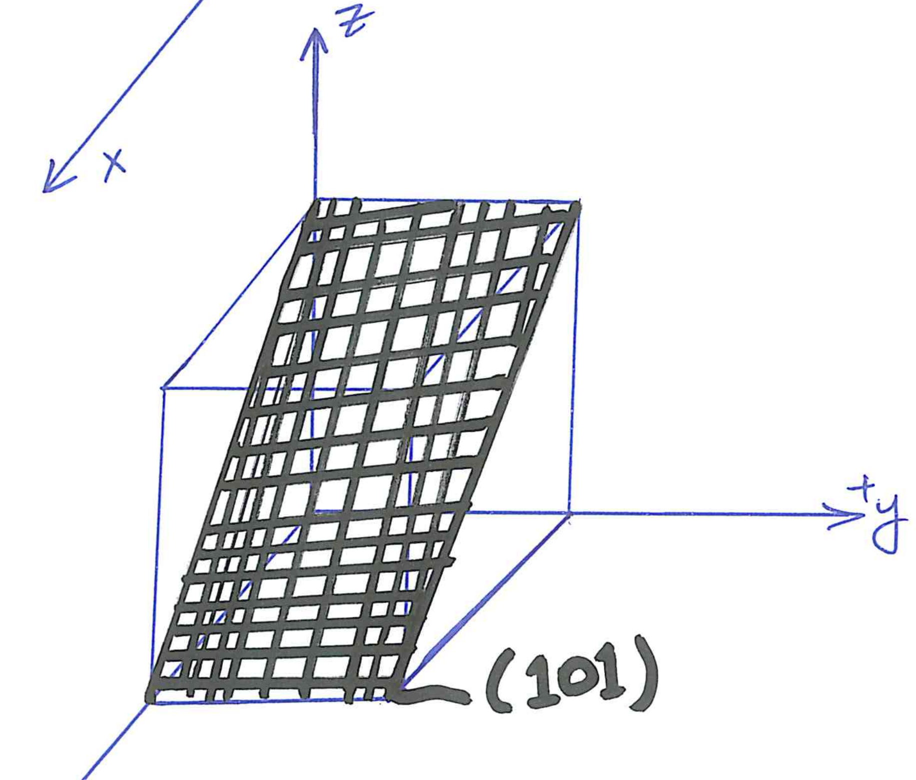
4)

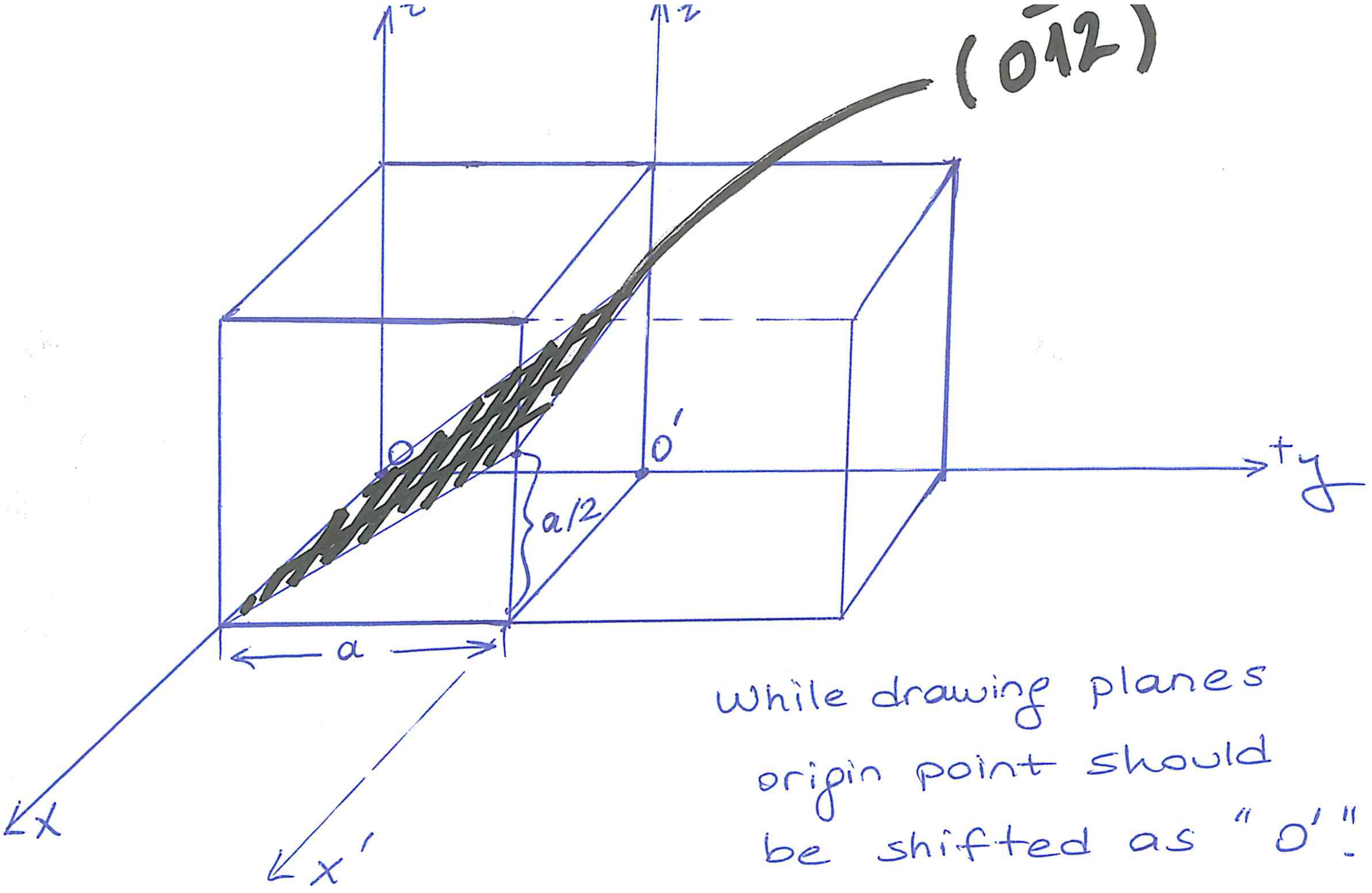


The directions in a unit cell.

[1$\bar{1}$0] , [111] , [110] , [120]


z
(001)
(0$\bar{1}\bar{1}$)
-y
O
+y
x


z
+y
(101)
x



While drawing planes origin point should be shifted as "O'"!

So, according to the new origin O', the intercepts are:

$x = \infty \qquad y = -1 \qquad z = \frac{1}{2}$

Reciprocals ; $\frac{1}{\infty} \qquad \frac{1}{-1} \qquad \frac{1}{\frac{1}{2}}$

$0 \qquad -1 \qquad 2$

Plane $(0\bar{1}2)$