# Fundamentals of Materials Science
# Homework 9, SS 2017

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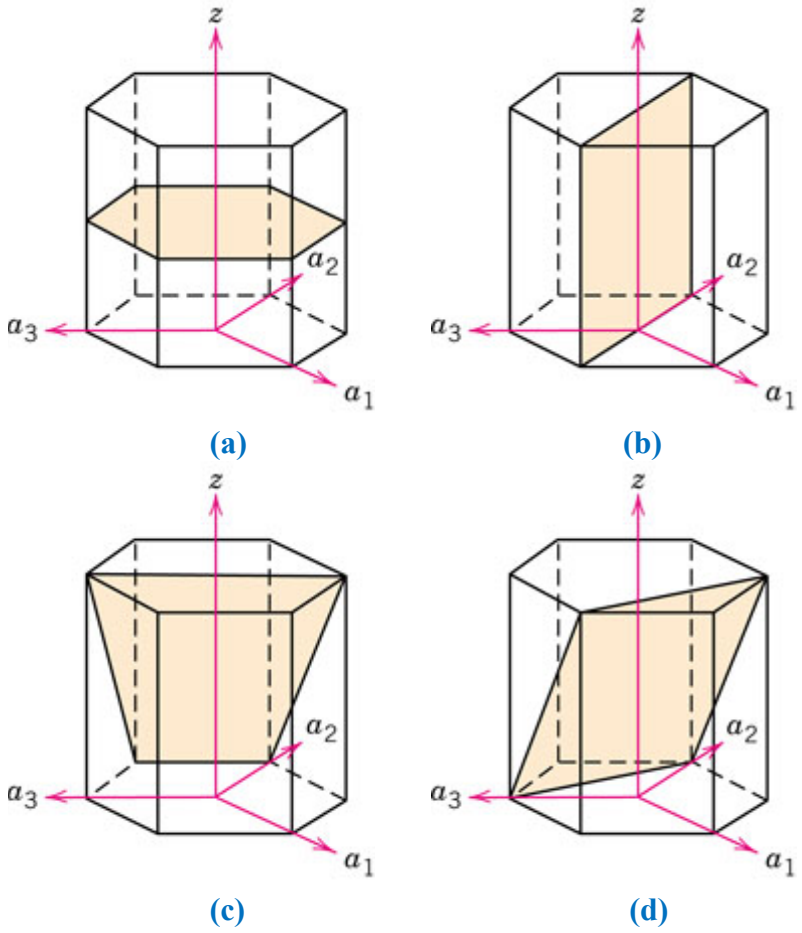
1. Determine the *Miller-Bravais* indices for the planes shown in the following unit cells:




***Solution***

**(a)**

| | *a1* | *a2* | *a3* | *z* |
|---|---|---|---|---|
| Intercepts | ∞a | ∞a | - | 1/2c |
| Intercepts in terms of a and c | ∞ | ∞ | - | 1/2 |
| Reciprocals to intercepts | 0 | 0 | 0 | 2 |
| Reduction | 0 | 0 | 0 | 1 |
| Enclosure | (0 0 0 1) | | | |

**(b)**

| | *a1* | *a2* | *a3* | *z* |
|---|---|---|---|---|
| Intercepts | a | ∞a | - | ∞c |
| Intercepts in terms of a and c | 1 | ∞ | - | ∞ |
| Reciprocals to intercepts | 1 | 0 | -1 | 0 |
| Reduction | 1 | 0 | -1 | 0 |
| Enclosure | $(1\ 0\ \bar{1}\ 0)$ | | | |

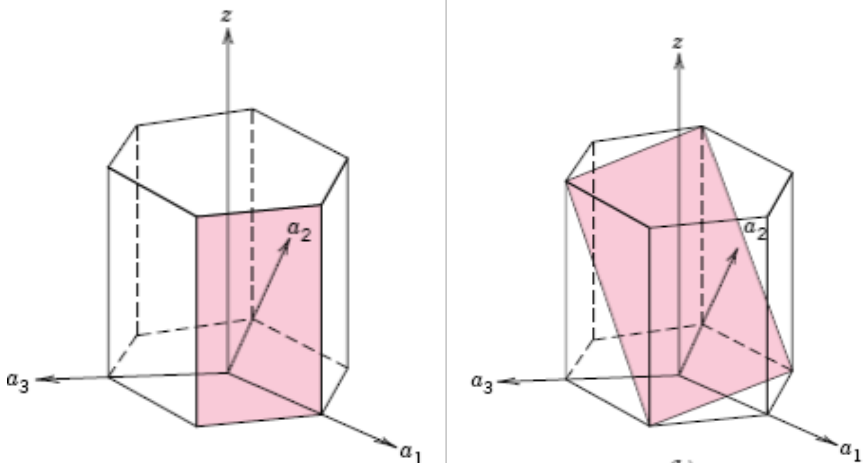
**(c)**

| | *a1* | *a2* | *a3* | *z* |
|---|---|---|---|---|
| Intercepts | -a | a | - | c |
| Intercepts in terms of a and c | -1 | **1** | - | 1 |
| Reciprocals to intercepts | -1 | 1 | 0 | 1 |
| Reduction | -1 | 1 | 0 | 1 |
| Enclosure | $(\bar{1}\ 1\ 0\ 1)$ | | | |

**(d)**

| | *a1* | *a2* | *a3* | *z* |
|---|---|---|---|---|
| Intercepts | -a/2 | a | - | c/2 |
| Intercepts in terms of a and c | -1/2 | 1 | - | 1/2 |
| Reciprocals to intercepts | -2 | 1 | 1 | 2 |
| Reduction | -2 | 1 | 1 | 2 |
| Enclosure | $(\bar{2}\ 1\ 1\ 2)$ | | | |

2. Determine the *Miller-Bravais* indices for the planes shown in the following unit cells:




**(a)** **(b)**

***Solution***

**(a)**

| | *a1* | *a2* | *a3* | *z* |
|---|---|---|---|---|
| Intercepts | a | -a | - | ∞c |
| Intercepts in terms of a and c | 1 | -1 | - | ∞ |
| Reciprocals to intercepts | 1 | -1 | 0 | 0 |
| Reduction | 1 | -1 | 0 | 0 |
| Enclosure | $(1\ \bar{1}\ 0\ 0)$ | | | |

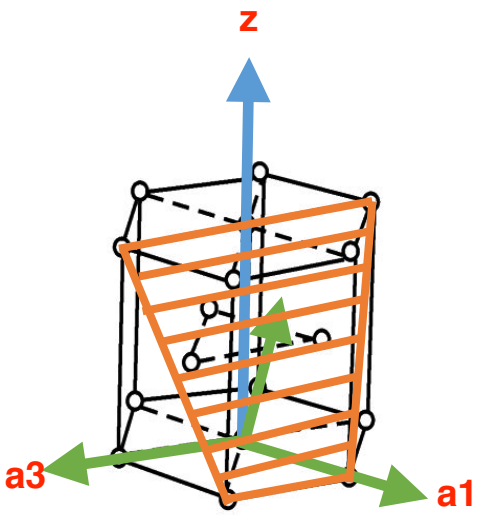
**(b)**

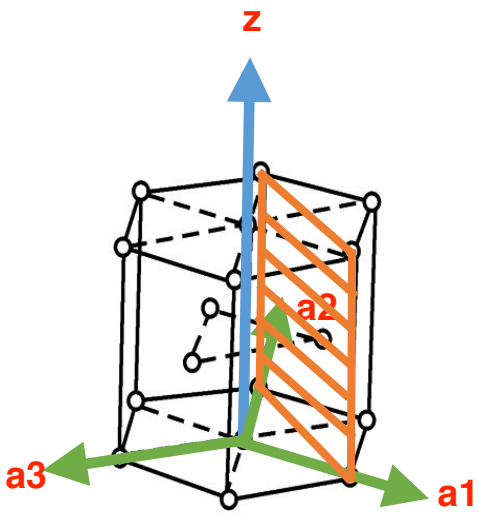
| | *a1* | *a2* | *a3* | *z* |
|---|---|---|---|---|
| Intercepts | a/2 | -a | - | 1/2c |
| Intercepts in terms of a and c | 1/2 | -1 | - | 1/2 |
| Reciprocals to intercepts | 2 | -1 | -1 | 2 |
| Reduction | 2 | -1 | -1 | 2 |
| Enclosure | $(2\ \bar{1}\ \bar{1}\ 2)$ | | | |

3. Sketch the $(1\bar{1}01)$ and $(11\bar{2}0)$ planes in a hexagonal unit cell.

***Solution***

$(1\bar{1}01)$ $(11\bar{2}0)$

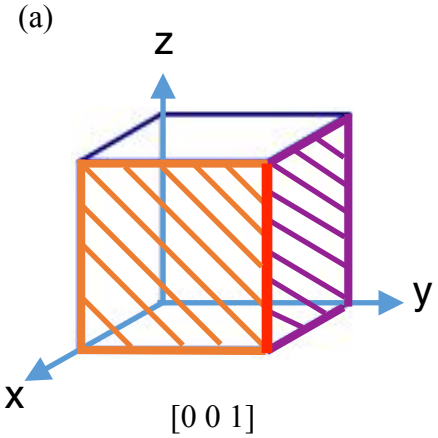



4. Cite the indices of the direction that results from the intersection of each of the following pairs of planes within a cubic crystal: **(a)** the $(100)$ and $(010)$ planes, **(b)** the $(111)$ and $(11\bar{1})$ planes, **(c)** the $(10\bar{1})$ and $(001)$ planes.

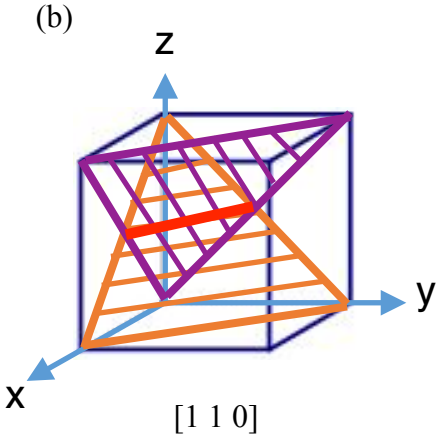
***Solution***

(a)



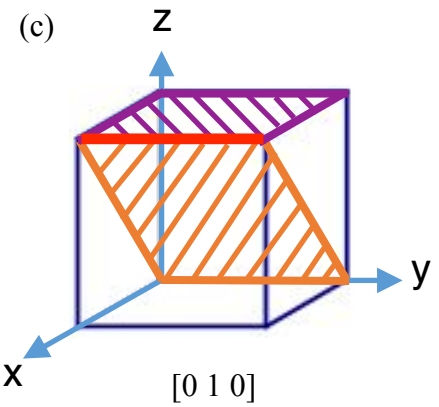

[0 0 1]

(b)




[1 1 0]

(c)




[0 1 0]

5. For the HCP crystal structure, show that the ideal c/a ratio is 1.633. Calculate the atomic packing fraction for the hexagonal close-packed crystal structure for which $c = a\sqrt{8/3}$. Remember that the base of the unit cell is a parallelogram.

***Solution***

$$APF_{HCP}=\frac{volume\ of\ atoms\ in\ a\ unit\ cell}{total\ unit\ cell\ volume}$$

$$=\frac{\frac{4}{3}\pi R^3\times 6}{3V_{para}}=\frac{8\pi R^3}{3\times(a\times\frac{\sqrt{3}}{2}a\times c)}$$

$$=\frac{16\pi R^3}{3\sqrt{3}\times\sqrt{\frac{8}{3}}\times a^3}=\frac{16\pi R^3}{6\sqrt{2}\times(2R)^3}=\frac{\pi}{3\sqrt{2}}$$

$$=0.74$$

6. Zirconium has an HCP crystal structure and a density of 6.51 g/cm$^3$.
   **(a)** What is the volume of its unit cell in cubic meters?
   **(b)** If the *c*/*a* ratio is 1.593, compute the values of *c* and *a*.

***Solution***

(a) *Known number*

Atomic weight of Zr: $A_{Zr}$=91.22amu

Because the crystal structure is HCP, n, the number of atoms per unit cell, is 6.

Furthermore, the atomic weight $A_{Zr}$ is given as 91.22amu. The density of Zr is given in the question, thus

$$V_{Zr}=\frac{n_{HCP}A_{Zr}}{\rho_{Zr}N_A}$$

$$V_{Zr}=\frac{(6\ atoms/unit\ cell)\times(91.22\ g/mol)}{(6.51\ g/cm^3)\times(6.022\times10^{23}\ atoms/mol)}$$

$$=1.40\times10^{-22}cm^3/unit\ cell$$

$$=1.40\times10^{-28}m^3/unit\ cell$$

(b) In HCP crystal structure, the volume of the unit cell is

$$V=3V_{para}=3a\times\frac{\sqrt{3}}{2}a\times c$$

$$=\frac{3\sqrt{3}}{2}a^2\times1.593a$$

$$=4.139a^3=1.40\times10^{-28}m^3/unit\ cell$$

Thus,

$$a=\sqrt[3]{\frac{1.40\times10^{-28}m^3}{4.139}}=3.234\times10^{-10}m=0.323nm$$

$$c=1.593a=0.515nm$$

7. Rhodium has an atomic radius of 0.1345 nm (1.345Å) and a density of 12.41 g/cm$^3$. Determine whether it has an FCC or BCC crystal structure.

***Solution***

*Known number*

Atomic weight of Rh: $A_{Rh}$=102.91amu

According to the equation,

$$\rho_{Rh}=\frac{nA_{Rh}}{VN_A}$$

If Rh has an FCC crystal structure,

$$\begin{aligned}\rho_{Rh}&=\frac{n_{FCC}A_{Rh}}{a_{FCC}^3N_A}\\&=\frac{(4\ atoms/unit\ cell)\times(102.91g/mol)}{(2\sqrt{2}\,R)^3\times(6.022\times10^{23}atoms)}\\&=\frac{(4\ atoms/unit\ cell)\times(102.91g/mol)}{(2\sqrt{2}\times0.1345\times10^{-7}cm)^3\times(6.022\times10^{23}atoms/mol)}\\&=12.41g/cm^3\end{aligned}$$

If Rh has a BCC crystal structure,

$$\begin{aligned}\rho_{Rh}&=\frac{n_{BCC}A_{Rh}}{a_{BCC}^3N_A}\\&=\frac{(2\ atoms/unit\ cell)\times(102.91g/mol)}{(\frac{4}{\sqrt{3}}R)^3\times(6.022\times10^{23}atoms)}\\&=\frac{(2\ atoms/unit\ cell)\times(102.91g/mol)}{(\frac{4}{\sqrt{3}}\times0.1345\times10^{-7}cm)^3\times(6.022\times10^{23}atoms/mol)}\\&=11.40g/cm^3\end{aligned}$$

Since the density of Rhodium is given as 12.41g/cm$^3$, so it has an FCC crystal structure.

8. Beryllium (Be) has an HCP unit cell for which the ratio of the lattice parameters c/a is 1.568. If the radius of the Be atom is 0.1143 nm, (a) determine the unit cell volume, and (b) calculate the theoretical density of Be and compare it with the literature value.

***Solution***

(a)

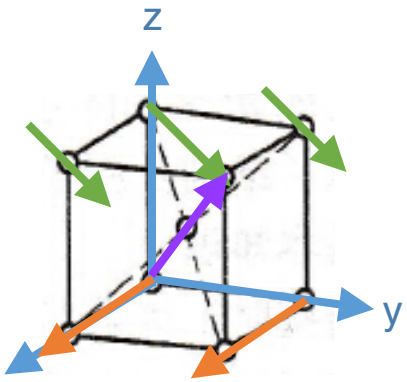
$$\begin{aligned}V_{HCP}&=3V_{para}=3a\times\frac{\sqrt{3}}{2}a\times c\\&=\frac{3\sqrt{3}}{2}a^2\times1.568a\\&=4.074a^3=4.074\times(2R)^3=4.074\times(2\times0.1143\times10^{-7}cm)^3\\&=4.867\times10^{-23}cm^3\end{aligned}$$

(b) *Known number*: Atomic weight of Be: $A_{Be}$=9.012amu

$$\begin{aligned}\rho_{Be}&=\frac{n_{HCP}A_{Be}}{V_{Be}N_A}\\&=\frac{(6\ atoms/unit\ cell)\times(9.012g/mol)}{(4.867\times10^{-23}cm^3)\times(6.022\times10^{23}atoms/mol)}\\&=1.845g/cm^3\end{aligned}$$

Thus, the theoretical density of Be is 1.845g/cm$^3$, and the literature value is 1.85g/cm$^3$.

9. Calculate and compare the linear densities for the <100>, <110> and <111> directions in a BCC unit cell. Which direction is the most close-packed (dense)?




<100>

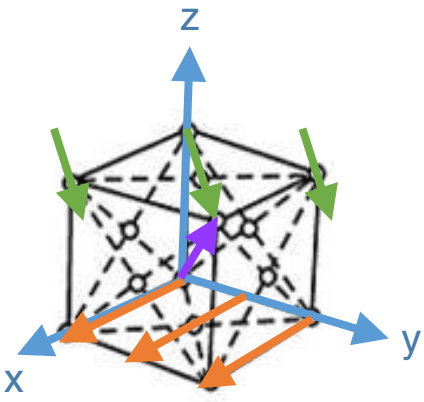
<110>

<111>

<100>: $d_{100}=4\sqrt{3}R/3=2.31R$
<110>: $d_{110}=4\sqrt{6}R/3=3.27R$
<111>: $d_{111}=2R$

Thus, the linear densities for the <111> directions is the most close-packed.

10. Calculate and compare the linear densities for the <100>, <110> and <111> directions in a FCC unit cell. Which direction is the most close-packed (dense)?




<100>

<110>

<111>

<100>: $d_{100}=2\sqrt{2}R$
<110>: $d_{110}=2R$
<111>: $d_{111}= 2\sqrt{6}R$

Thus, the linear densities for the <110> directions is the most close-packed.

11. Suppose that FCC rhodium is produced as a 1-mm thick sheet, with the (111) plane parallel to the surface of the sheet. How many (111) interplanar spacings $d_{111}$ thick is the sheet? See Appendices in your textbook for necessary data.

***Solution***

*Known number*

Lattice parameter of Rh: 0.38044nm

Since an interplanar spacing is equal to

$$d_{111}=\frac{lattice\ \ parameter}{\sqrt{h^2+k^2+l^2}}$$

$$=\frac{0.38044nm}{\sqrt{1^2+1^2+1^2}}=0.21965nm$$

Thus, the number of interplanar spacings in a 1-mm thick sheet $n$ is equal to

$$n=\frac{1mm}{d_{111}}=\frac{1\times10^6nm}{0.21965nm}=4.55270\times10^6$$

12. Determine the minimum radius of an atom that will just fit into (a) the tetrahedral interstitial site in FCC nickel; and (b) the octahedral interstitial site in BCC lithium.

***Solution***

*Known numbers*

Lattice parameter of Ni: 0.35236nm

Lattice parameter of Li: 0.35089nm

r+/r- range: tetrahedron 0.225~0.414

octahedron 0.414~0.732

(a)For the tetrahedral site in FCC nickel,

$$r_{Ni}=\frac{a}{2\sqrt{2}}=\frac{0.35236nm}{2\sqrt{2}}=0.12360nm$$

According to the question, $r_{min}/r_{Ni}=0.225$

Thus, $r_{min}=r_{Ni}\times 0.225=(0.12360nm)\times 0.225=0.02781nm$

(b)For the octahedron site in BCC lithium,

$$r_{Li}=\frac{a}{\frac{4}{\sqrt{3}}}=\frac{0.35089nm}{\frac{4}{\sqrt{3}}}=0.15194nm$$

According to the question, $r_{min}/r_{Li}=0.414$

Thus, $r_{min}=r_{li}\times 0.414=(0.15194nm)\times 0.414=0.06290nm$

13. The atomic packing fraction for the FCC crystal structure is 0.74. This is the densest arrangement of atoms achievable in three dimensions when all atoms have the same radius *R*. If atoms in the hard sphere model occupy 74% of the volume of the unit cell, then the other 26% is empty space. Imagine that the empty spaces located at the center of each edge and at the body–centered position of the FCC unit cell are filled with smaller spheres of radius *r* such that $r = 0.414R$. The smaller atoms fit perfectly in between the atoms of radius *R*. (a) By counting in the usual way, how many atoms of radius *r* are there per FCC unit cell? (b) What are the coordinates of these atoms of radius *r*? Do not double count atoms. Provide the same number of coordinates as the number of atoms of radius *r* per unit cell. (c) What is the atomic packing fraction for this structure?

***Solution***

(a)Numbers of atoms of radius *r* per unit cell: $N=8\times\frac{1}{4}+1=3$

(b) The coordinates of these atoms of radius *r*:

Underside: (1/2, 0, 0), (0, 1/2, 0), (1, 1/2, 0), (1/2, 1, 0);

Upside: (1/2, 0, 1), (0, 1/2, 1), (1, 1/2, 1), (1/2, 1, 1);

Center: (1/2, 1/2, 1/2)

(c)

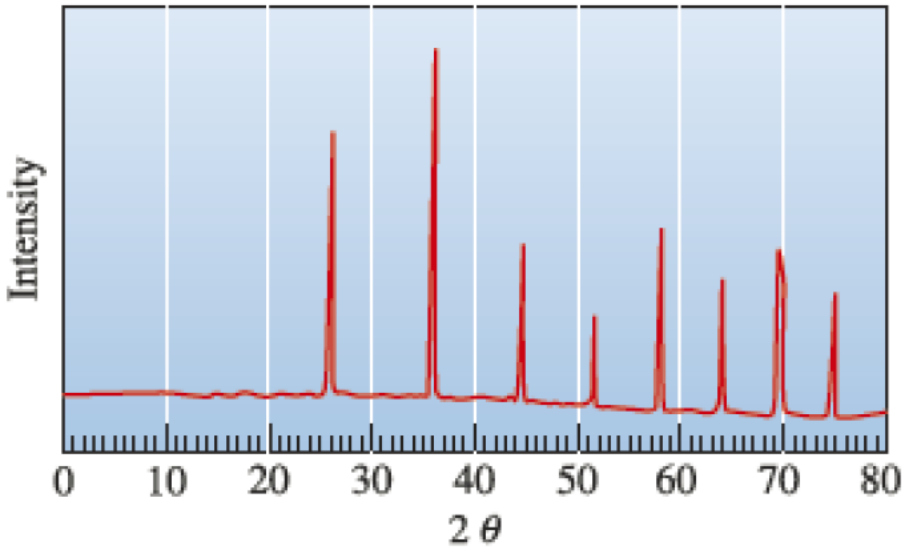
$$APF=\frac{volume\ of\ atoms\ in\ a\ unit\ cell}{total\ unit\ cell\ volume}$$

$$=\frac{4\times\frac{4}{3}\pi R^3+3\times\frac{4}{3}\pi r^3}{a^3}$$

$$=\frac{4\times\frac{4}{3}\pi R^3+3\times\frac{4}{3}\pi(0.414R)^3}{(2\sqrt{2}\,R)^3}$$

$$=0.78$$

14. The Figure below shows the results of an x-ray diffraction experiment in the form of the intensity of the diffracted peak versus the $2\theta$ diffraction angle. If x-rays with a wavelength of 0.07107 nm are used, determine (a) the crystal structure of the metal; (b) the indices of the planes that produce each of the peaks; and (c) the lattice parameter of the metal.




***Solution***

According to the equation, $n\lambda=2d_{hkl}sin2\theta$

$$sin^2\theta=\frac{\lambda^2}{4a^2}m$$

Assuming that n=1, 8 peaks corresponding 8 different values of $2\theta$,

| | $2\theta$ | $sin^2\theta$ | $m_i/m_1$ |
|---|---|---|---|
| 1 | 25.5° | 0.0487 | 1 |
| 2 | 36.0° | 0.0955 | 2 |
| 3 | 44.5° | 0.1434 | 3 |
| 4 | 51.5° | 0.1887 | 4 |
| 5 | 58.0° | 0.2350 | 5 |
| 6 | 64.5° | 0.2847 | 6 |
| 7 | 70.0° | 0.3290 | 7 |
| 8 | 75.5° | 0.3748 | 8 |

(a)

| 衍射线顺序号 | 简单立方 | | | 体心立方 | | | 面心立方 | | | 金刚石立方 | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | HKL | $m$ | $m_i/m_1$ | HKL | $m$ | $m_i/m_1$ | HKL | $m$ | $m_i/m_1$ | HKL | $m$ | $m_i/m_1$ |
| 1 | 100 | 1 | 1 | 110 | 2 | 1 | 111 | 3 | 1 | 111 | 3 | 1 |
| 2 | 110 | 2 | 2 | 200 | 4 | 2 | 200 | 4 | 1.33 | 220 | 8 | 2.66 |
| 3 | 111 | 3 | 3 | 211 | 6 | 3 | 220 | 8 | 2.66 | 311 | 11 | 3.67 |
| 4 | 200 | 4 | 4 | 220 | 8 | 4 | 311 | 11 | 3.67 | 400 | 16 | 5.33 |
| 5 | 210 | 5 | 5 | 310 | 10 | 5 | 222 | 12 | 4 | 331 | 19 | 6.33 |
| 6 | 211 | 6 | 6 | 222 | 12 | 6 | 400 | 16 | 5.33 | 422 | 24 | 8 |
| 7 | 220 | 8 | 8 | 321 | 14 | 7 | 331 | 19 | 6.33 | 333, 511 | 27 | 9 |
| 8 | 300, 221 | 9 | 9 | 400 | 16 | 8 | 420 | 20 | 6.67 | 440 | 32 | 10.67 |
| 9 | 310 | 10 | 10 | 411, 330 | 18 | 9 | 422 | 24 | 8 | 531 | 35 | 11.67 |
| 10 | 311 | 11 | 11 | 420 | 20 | 10 | 333, 511 | 27 | 9 | 620 | 40 | 13.33 |

Thus, the crystal structure of the metal is BCC.

(b)

| Number of peaks | Indices of the planes |
|---|---|
| 1 | (1 1 0) |
| 2 | (2 0 0) |
| 3 | (2 1 1) |
| 4 | (2 2 0) |
| 5 | (3 1 0) |
| 6 | (2 2 2) |
| 7 | (3 2 1) |
| 8 | (4 0 0) |

(c)

| # | $2\theta/°$ | h | k | l | $d=\lambda/2\sin\theta$ | $a=d\sqrt{h^2+k^2+l^2}$ |
|---|---|---|---|---|---|---|
| 1 | 25.5 | 1 | 1 | 0 | 0.162520613672182 | 0.229838856020399 |
| 2 | 36 | 2 | 0 | 0 | 0.116069932275111 | 0.232139864550222 |
| 3 | 44.5 | 2 | 1 | 1 | 0.0947243931831716 | 0.23202642949354 |
| 4 | 51.5 | 2 | 2 | 0 | 0.0825580261704366 | 0.233509360585969 |
| 5 | 58 | 3 | 1 | 0 | 0.0739808011781339 | 0.233947834846971 |
| 6 | 64.5 | 2 | 2 | 2 | 0.0672137301351131 | 0.232835191120478 |
| 7 | 70 | 3 | 2 | 1 | 0.0625302260296837 | 0.23396668212061 |
| 8 | 75.5 | 4 | 0 | 0 | 0.0585829166195756 | 0.234331666478303 |
| | Average | | | | | 0.232824485652061 |

Thus, the average of the lattice parameter of the metal is 0.2328nm.