

# 2026년도 1학기 에너지소자실험

**신기현 (조교: 오장현)**

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# Schedule

1	5월 12일	보고서/발표 작성 요령 + 이론	신기현
2	5월 19일	실습 (1조, 2조)	오장현
3	5월 26일	실습 (3조, 4조)	오장현
4	6월 2일	휴강	-
5	6월 9일	발표평가	신기현

**XRD Simulation : 오장현 조교에게 문의 ([wkdgus0313@gmail.com](mailto:wkdgus0313@gmail.com))**

**강의자료 및 상세내용들은 홈페이지 참고 ([themad.hanbat.ac.kr](http://themad.hanbat.ac.kr))**

# Team

## 1. Team01 (5/19)

방병조, 전진영, 최성민, 최은서, 민유빈

## 2. Team02 (5/19)

이찬복, 방현우, 남선미, 정소영, 박서연

## 3. Team03 (5/26)

임종범, 심태준, 오예원, 서지혜, 전영은

## 4. Team04 (5/26)

한준희, 명건우, 최현주, 길지수

# Evaluation

## 1. 보고서는 **개인** 제출 - 6/16일 까지 (이후 제출 0점)

- 양식 (양식은 홈페이지 참고) 미활용시 감점 (-5)
- 팀원끼리는 토의만 진행 → 보고서 내용이 동일할 경우 모두 0점
- 보고서의 포맷 및 퀄리티 (예쁘게 깔끔하게) 가 좋을 경우 가산점 (+5) 반대의 경우 (-5)
- 보고서 표지 만들 것 (+5)

## 2. 발표는 **팀별로 (10분 분량 준비)** - 6/9일

- 발표자에게는 가산점 (단, 발표내용을 적어서 읽을 경우 가산점 X) (+5)
- 발표자료의 포맷 및 퀄리티 (예쁘게, 깔끔하게) 가 좋을 경우 가산점 (+5) 반대의 경우 (-5)
- 발표태도가 뛰어나면 가산점 (+3)
- 질문을 할 경우에 가산점 (+5)

# Importance of Appearance

**보기에 좋은 떡이 먹기도 좋다**

**빛 좋은 개살구**

**여우와 신 포도 (“저 포도는 어차피 신 포도일 거야”)**

**뚝배기 보다 장맛이 좋다**

# Importance of Appearance

**보기에 좋은 떡이 먹기도 좋다**

**빛 좋은 개살구**  
**(먹어봐야 안다)**

**여우와 신 포도 (“저 포도는 어차피 신 포도일 거야”)**

**뚝배기 보다 장맛이 좋다**  
**(먹어봐야 안다)**

# Fundamentals of XRD

X선 회절 = XRD (X-ray Diffraction)

X-ray wavelength : 0.01 ~ 10 nm

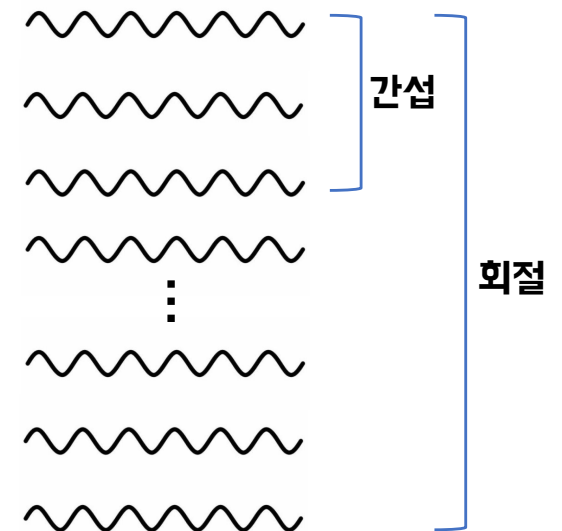
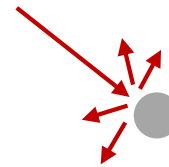
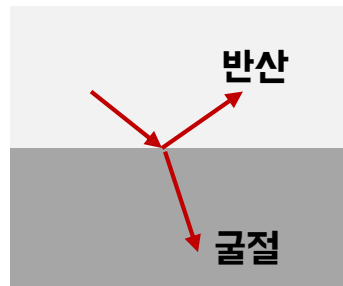
Scale of atom : 1 Å = 0.1 nm

CuK $\alpha$  = 1.5406 Å

반사, 굴절,

'산란',

'회절', 간섭



# Bragg's Law

- Diffraction (회절)
  - 파동이 좁은 틈을 지날 때 진행 경로가 퍼져 나가는 현상
  - 상쇄/보강간섭에 의해 회절무늬가 나타난다.

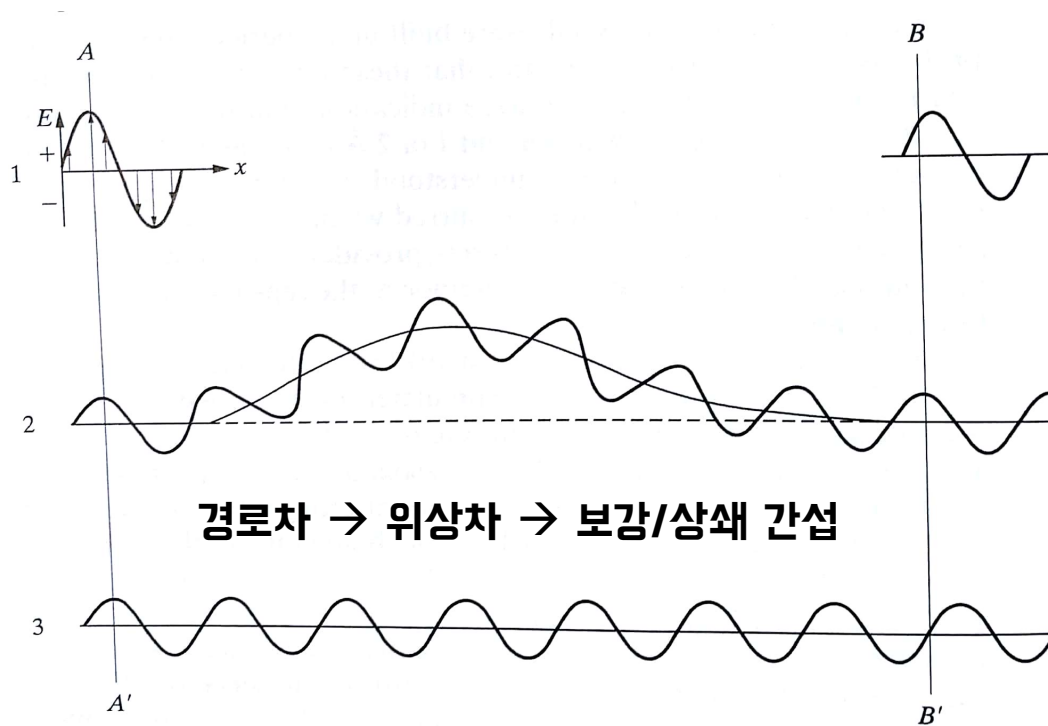
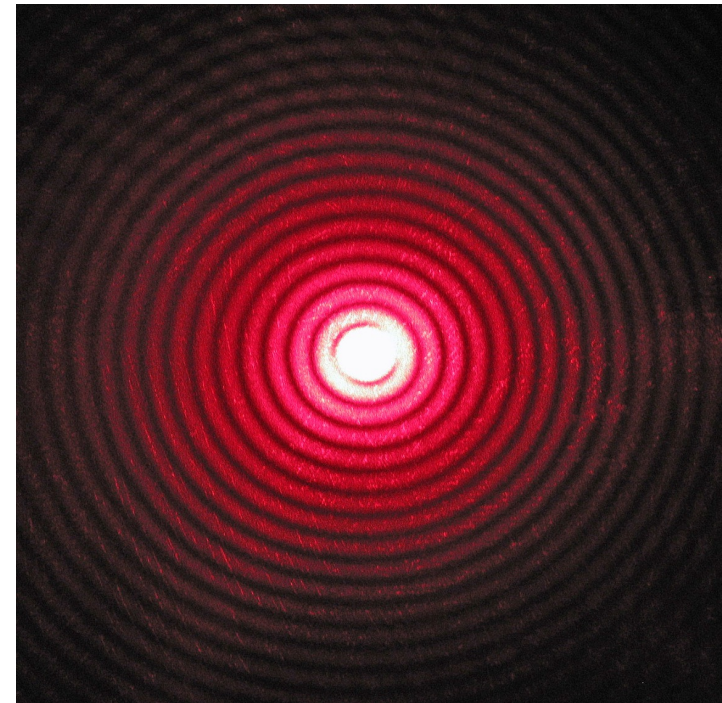
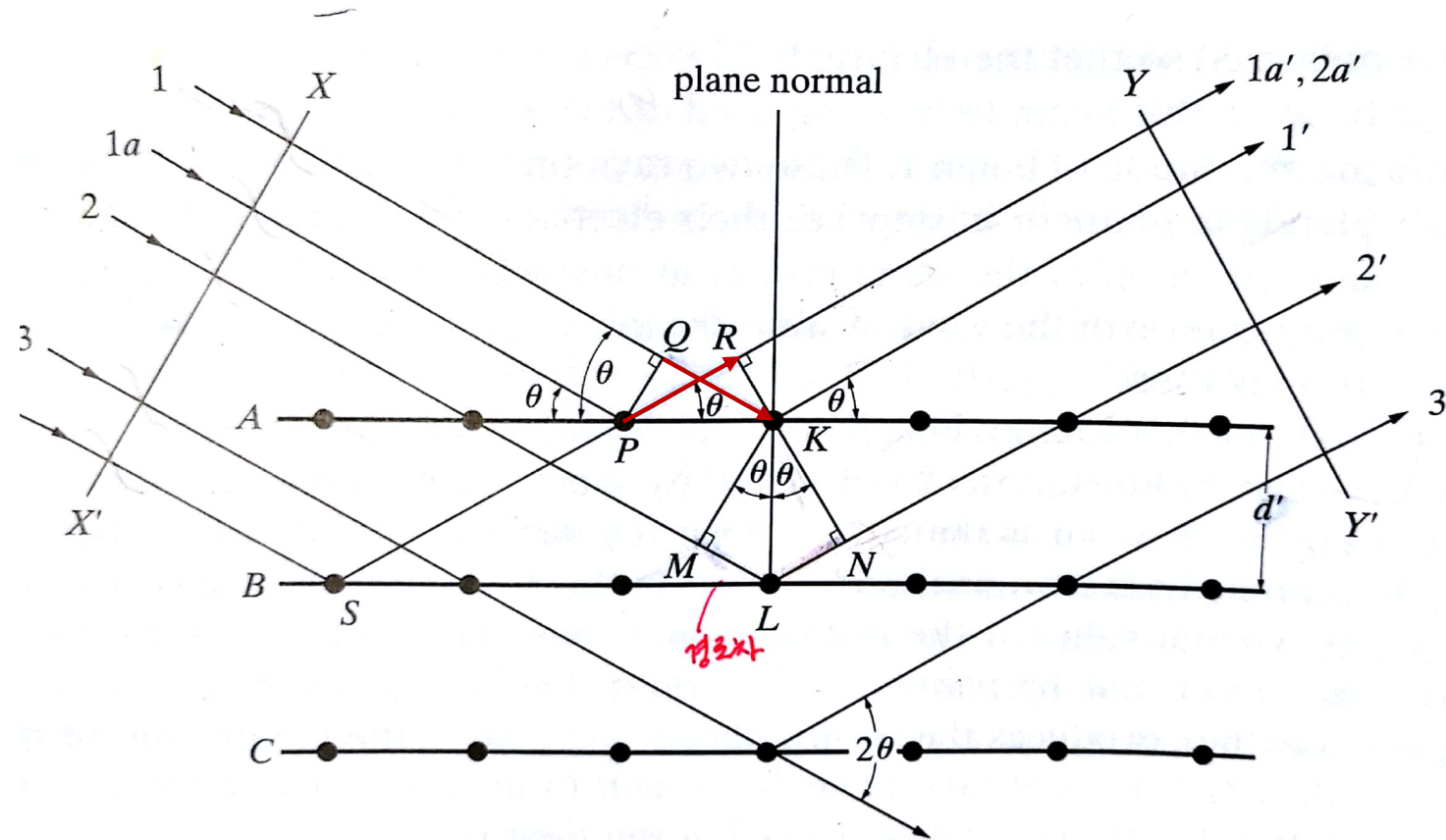


Figure 3-1 Effect of path difference on relative phase.



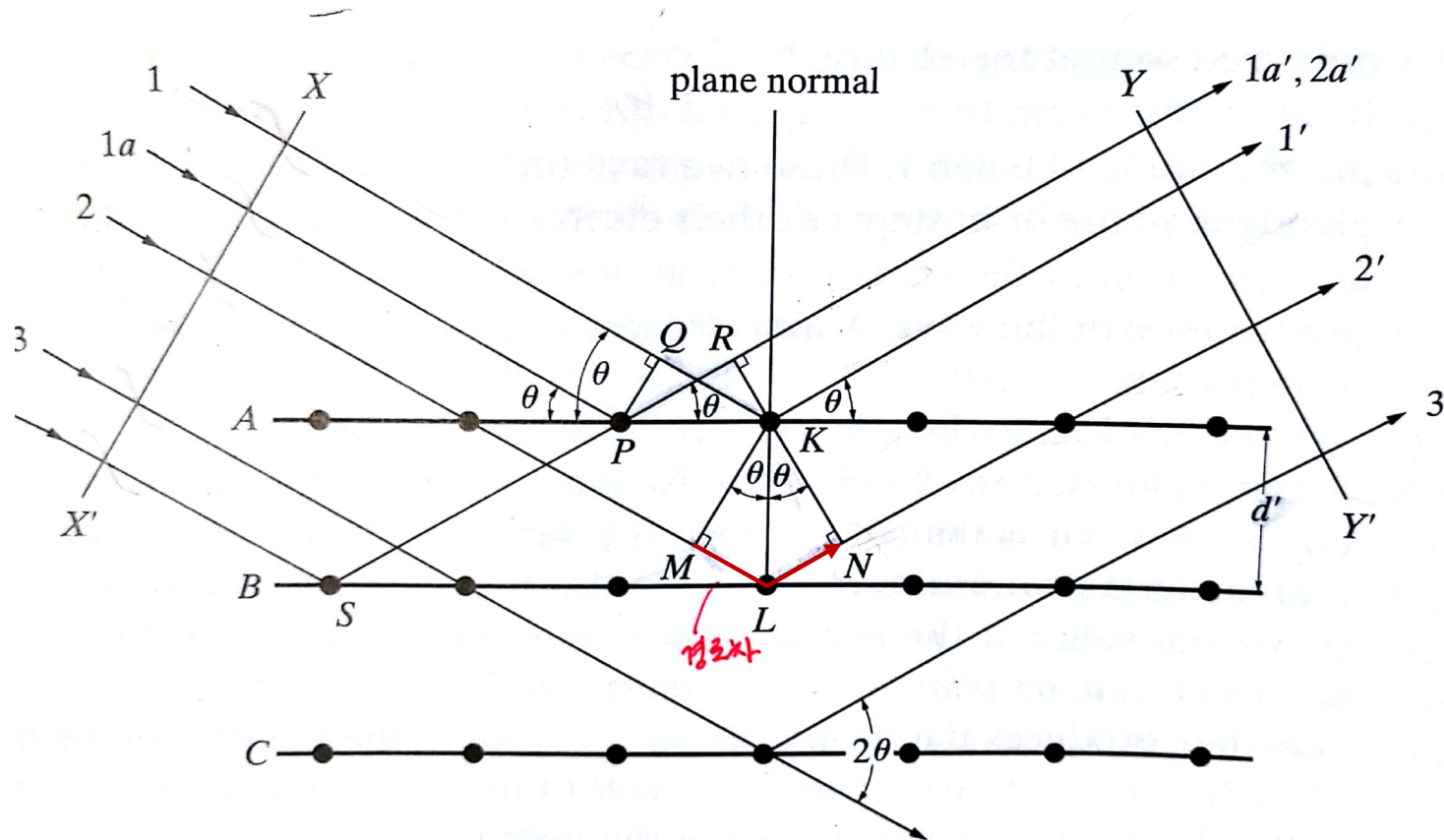
# Bragg's Law



조건 : 면간거리  $d'$  의 결정. 파장  $\lambda$  의 X-ray 가  $\theta$  각으로 조사되었을 때



# Bragg's Law



2. 서로 다른 면에서는 경로 차가 = 파장의 정수 배 일 때 → 회절 (1-1', 2-2'의 경우)

$$LM + LN(\text{경로차}) = d' \sin\theta + d' \sin\theta = n\lambda$$

$$n\lambda = 2d' \sin\theta$$

$n$  : order of diffraction → 1<sup>st</sup> order 사용

# Diffraction Direction

## 결정격자별 (hkl) 면의 peak 의 위치 ( $\theta$ )

$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)}{a^2} \quad \lambda = 2d \sin \theta$$

$$\sin^2 \theta = \frac{\lambda^2}{4a^2} (h^2 + k^2 + l^2)$$

### PLANE SPACINGS

The value of  $d$ , the distance between adjacent planes in the set  $(hkl)$ , may be found from the following equations.

Cubic: 
$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Tetragonal: 
$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

Hexagonal: 
$$\frac{1}{d^2} = \frac{4}{3} \left( \frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$$

Rhombohedral:

$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2 \alpha + 2(hk + kl + hl)\cos^2 \alpha - \cos \alpha}{a^2(1 - 3\cos^2 \alpha + 2\cos^3 \alpha)}$$

Orthorhombic: 
$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Monoclinic: 
$$\frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left( \frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right)$$

Triclinic: 
$$\frac{1}{d^2} = \frac{1}{V^2} (S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl)$$

In the equation for triclinic crystals,

$V$  = volume of unit cell (see below),

$$S_{11} = b^2c^2\sin^2 \alpha,$$

$$S_{22} = a^2c^2\sin^2 \beta,$$

$$S_{33} = a^2b^2\sin^2 \gamma,$$

$$S_{12} = abc^2(\cos \alpha \cos \beta - \cos \gamma),$$

$$S_{23} = a^2bc(\cos \beta \cos \gamma - \cos \alpha),$$

$$S_{13} = ab^2c(\cos \gamma \cos \alpha - \cos \beta).$$

# Intensity of Diffraction

Structure factor : 결정내 원자들에 의해 scattering 된 beam의 intensity

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

$hkl$  면에서의  $uvw$  위치의 원자들에 의한 scattering beam의 강도

$f_n$  : atomic scattering factor (원자별로 다름)

## Atomic Scattering Factors

$\frac{\sin \theta}{\lambda} (\text{\AA}^{-1})$	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	
H	1	0.81	0.48	0.25	0.13	0.07	0.04	0.03	0.02	0.01	0.00	0.00	0.00	
He	2	1.88	1.46	1.05	0.75	0.52	0.35	0.24	0.18	0.14	0.11	0.09	0.09	
Li <sup>+</sup>	2	1.96	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4	0.3	0.3	0.3	
Li	3	2.2	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4	0.3	0.3	0.3	
Be <sup>+2</sup>	2	2.0	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7	0.6	0.5	0.5	
Be	4	2.9	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7	0.6	0.5	0.5	
B <sup>+3</sup>	2	1.99	1.9	1.8	1.7	1.6	1.4	1.3	1.2	1.0	0.9	0.7	0.7	
B	5	3.5	2.4	1.9	1.7	1.5	1.4	1.2	1.2	1.0	0.9	0.7	0.7	
C	6	4.6	3.0	2.2	1.9	1.7	1.6	1.4	1.3	1.16	1.0	0.9	0.9	
N <sup>+5</sup>	2	2.0	2.0	1.9	1.9	1.8	1.7	1.6	1.5	1.4	1.3	1.16	1.16	
N <sup>+3</sup>	4	3.7	3.0	2.4	2.0	1.8	1.66	1.56	1.49	1.39	1.28	1.17	1.17	
N	7	5.8	4.2	3.0	2.3	1.9	1.65	1.54	1.49	1.39	1.29	1.17	1.17	
O	8	7.1	5.3	3.9	2.9	2.2	1.8	1.6	1.5	1.4	1.35	1.26	1.26	
O <sup>-2</sup>	10	8.0	5.5	3.8	2.7	2.1	1.8	1.5	1.5	1.4	1.35	1.26	1.26	
F	9	7.8	6.2	4.45	3.35	2.65	2.15	1.9	1.7	1.6	1.5	1.35	1.35	
F <sup>-</sup>	10	8.7	6.7	4.8	3.5	2.8	2.2	1.9	1.7	1.55	1.5	1.35	1.35	
Ne	10	9.3	7.5	5.8	4.4	3.4	2.65	2.2	1.9	1.65	1.55	1.5	1.5	
Na <sup>+</sup>	10	9.5	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95	1.75	1.6	1.6	
Na	11	9.65	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95	1.75	1.6	1.6	
Mg <sup>+2</sup>	10	9.75	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2	2.0	1.8	1.8	
Mg	12	10.5	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2	2.0	1.8	1.8	
Al <sup>+3</sup>	10	9.7	8.9	7.8	6.65	5.5	4.45	3.65	3.1	2.65	2.3	2.0	2.0	
Al	13	11.0	8.95	7.75	6.6	5.5	4.5	3.7	3.1	2.65	2.3	2.0	2.0	
Si <sup>+4</sup>	10	9.75	9.15	8.25	7.15	6.05	5.05	4.2	3.4	2.95	2.6	2.3	2.3	
Si	14	11.35	9.4	8.2	7.15	6.1	5.1	4.2	3.4	2.95	2.6	2.3	2.3	
P <sup>+5</sup>	10	9.8	9.25	8.45	7.5	6.55	5.65	4.8	4.05	3.4	3.0	2.6	2.6	
P	15	12.4	10.0	8.45	7.45	6.5	5.65	4.8	4.05	3.4	3.0	2.6	2.6	
P <sup>-3</sup>	18	12.7	9.8	8.4	7.45	6.5	5.65	4.85	4.05	3.4	3.0	2.6	2.6	
S <sup>+6</sup>	10	9.85	9.4	8.7	7.85	6.85	6.05	5.25	4.5	3.9	3.35	2.9	2.9	
S	16	13.6	10.7	8.95	7.85	6.85	6.0	5.25	4.5	3.9	3.35	2.9	2.9	
S <sup>-2</sup>	18	14.3	10.7	8.9	7.85	6.85	6.0	5.25	4.5	3.9	3.35	2.9	2.9	
Cl	17	14.6	11.3	9.25	8.05	7.25	6.5	5.75	5.05	4.4	3.85	3.35	3.35	
Cl <sup>-</sup>	18	15.2	11.5	9.3	8.05	7.25	6.5	5.75	5.05	4.4	3.85	3.35	3.35	
A	18	15.9	12.6	10.4	8.7	7.8	7.0	6.2	5.4	4.7	4.1	3.6	3.6	
K <sup>+</sup>	18	16.5	13.3	10.8	8.85	7.75	7.05	6.44	5.9	5.3	4.8	4.2	4.2	
K	19	16.5	13.3	10.8	9.2	7.9	7.1	6.44	5.9	5.2	4.6	4.2	3.7	3.3
Ca <sup>+2</sup>	18	16.8	14.0	11.5	9.3	8.1	7.35	6.7	6.2	5.7	5.1	4.6	4.6	4.6
Ca	20	17.5	14.1	11.4	9.7	8.4	7.3	6.3	5.6	4.9	4.5	4.0	3.6	3.6
Sc <sup>+3</sup>	18	16.7	14.0	11.4	9.4	8.3	7.6	6.9	6.4	5.8	5.35	4.85	4.85	4.85
Sc	21	18.4	14.9	12.1	10.3	8.9	7.7	6.7	5.9	5.3	4.7	4.3	3.9	3.9
Ti <sup>+4</sup>	18	17.0	14.4	11.9	9.9	8.5	7.85	7.3	6.7	6.15	5.65	5.05	5.05	5.05
Ti	22	19.3	15.7	12.8	10.9	9.5	8.2	7.2	6.3	5.6	5.0	4.6	4.2	4.2
V	23	20.2	16.6	13.5	11.5	10.1	8.7	7.6	6.7	5.9	5.3	4.9	4.4	4.4
Cr	24	21.1	17.4	14.2	12.1	10.6	9.2	8.0	7.1	6.3	5.7	5.1	4.6	4.6
Mn	25	22.1	18.2	14.9	12.7	11.1	9.7	8.4	7.5	6.6	6.0	5.4	4.9	4.9

# Intensity of Diffraction

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

SC : 원자위치 (0,0,0)

$$F_{hkl} = f e^{2\pi i(0)} = f \rightarrow \text{모든 면}$$

BCC : 원자위치 (0,0,0), (1/2,1/2,1/2)

$$F_{hkl} = f e^{2\pi i(0)} + f e^{2\pi i(\frac{h}{2} + \frac{k}{2} + \frac{l}{2})} = f[1 + e^{\pi i(h+k+l)}]$$

$$e^{\pi i(h+k+l)} = \cos \pi(h+k+l) + i \sin \pi(h+k+l)$$

$$h+k+l = \text{짝수} \rightarrow 2f$$

$$h+k+l = \text{홀수} \rightarrow 0 \rightarrow \text{No diffraction}$$

# Intensity of Diffraction

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$

FCC : 원자위치 (0,0,0), (0,1/2,1/2), (1/2,0,1/2), (1/2,1/2,0)

$$F_{hkl} = f[1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)}]$$

$h + k + l = \text{unmixed (모두 홀수/모두 짝수)} \rightarrow 4f$

$h + k + l = \text{mixed} \rightarrow 0 \rightarrow \text{No diffraction}$

# Determination of Crystal Structure

## Crystal Structure

## Diffraction Pattern

Unit Cell

Line Position

Atom Position

Line Intensity

Kind of Atom

Line relative intensity

$$\sin^2\theta = \frac{\lambda^2}{4a^2} (h^2 + k^2 + l^2)$$

**Peak position by crystal structure**

$$F_{hkl} = \sum_1^N f_n e^{2\pi i(hu_n + kV_n + lW_n)}$$

**Peak intensity by atomic position in unit cell**

# Connecting Server



mobaxterm



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MobaXterm

<https://mobaxterm.mobatek.net>

[MobaXterm free Xserver and tabbed SSH client for Windows](#)



설치

**MobaXterm** X server and SSH client. **MobaXterm** is your ultimate toolbox for remote computing.

In a single Windows application, it provides loads of functions that ...

## Download

Free X server for Windows with tabbed SSH terminal, telnet ...

## Download Home Edition

Changelog. Version 24.1 (2024-04-26). Improvement: the ...

## Features

MobaXterm allows you to launch remote sessions. You can ...

## Demo

Free X server for Windows with tabbed SSH terminal, telnet ...

## Plugins

Free X server for Windows with tabbed SSH terminal, telnet ...

[More results from mobatek.net »](#)

# Connecting Server

The screenshot displays the MobaXterm interface. The main window title is "MobaXterm". The menu bar includes "Terminal", "Sessions", "View", "X server", "Tools", "Games", "Settings", "Macros", and "Help". The toolbar contains icons for "Session", "Servers", "Tools", "Games", "Sessions", "View", "Split", "MultiExec", "Tunneling", "Packages", "Settings", and "Help". The "Session" icon is highlighted with a red box, and a red arrow points from it to the "Session settings" dialog box.

Host: themad.hanbat.ac.kr  
Username: team01 ~ team 04  
PW: n8318

**Session settings**

SSH Telnet Rsh Xdmcp RDP VNC FTP SFTP Serial File Shell Browser Mosh Aws S3 WSL

**Basic SSH settings**

Remote host \* themad.hanbat.ac.kr  Specify username team01 Port 22

**Advanced SSH settings** Terminal settings Network settings Bookmark settings

X11-Forwarding  Compression Remote environment: Interactive shell

Execute command:   Do not exit after command ends

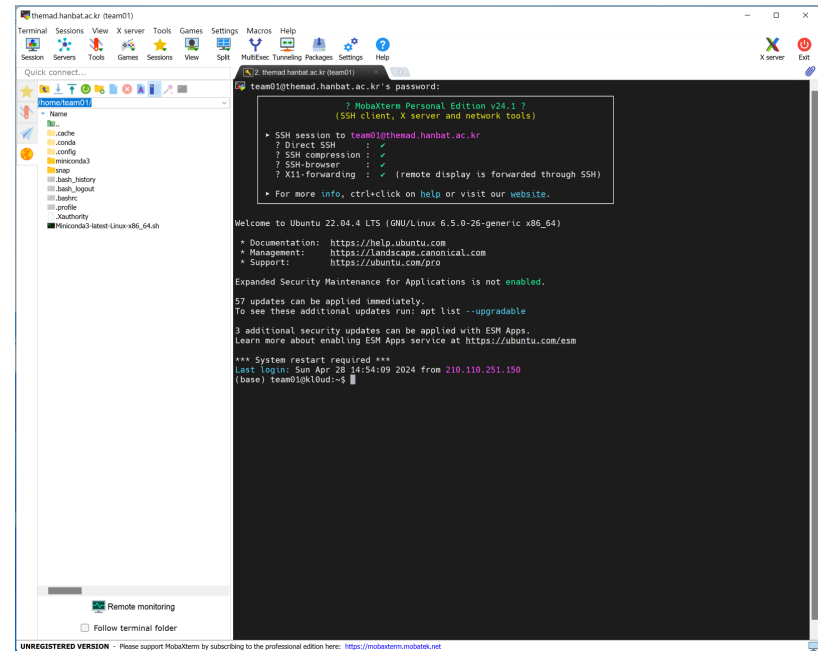
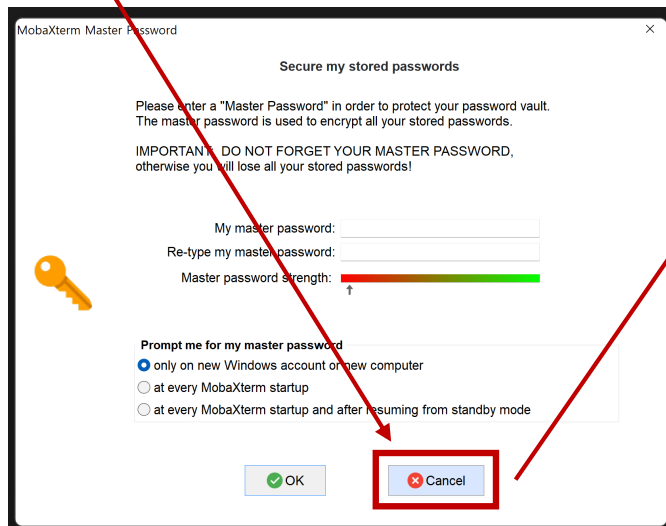
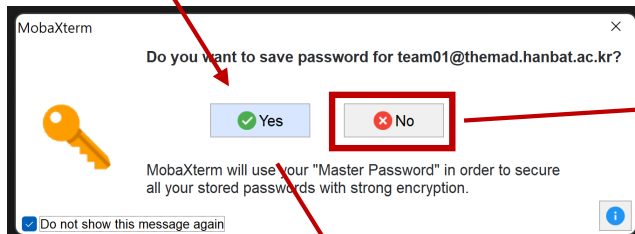
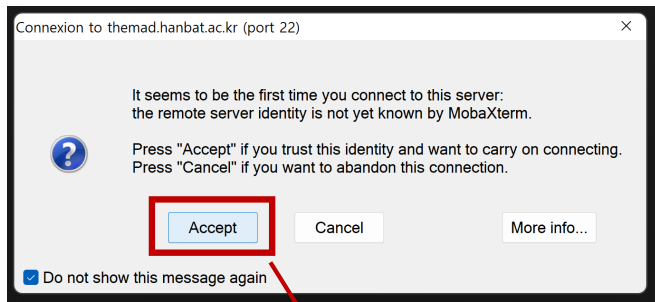
SSH-browser type: SFTP protocol  Follow SSH path (experimental)

Use private key

Execute macro at session start: <none>

UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: <https://mobaxterm.mobatek.net>

# Connecting Server



# Connecting Server

themad.hanbat.ac.kr (team01)

Terminal Sessions View X server Tools Games Settings Macros Help

Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help

Quick connect...

/home/team01/

- Name
- ..
- .cache
- .conda
- .config
- miniconda3
- snap
- .bash\_history
- .bash\_logout
- .bashrc
- .profile
- .Xauthority
- Miniconda3-latest-Linux-x86\_64.sh

team01@themad.hanbat.ac.kr's password:

```
? MobaXterm Personal Edition v24.1 ?  
(SSH client, X server and network tools)  
▶ SSH session to team01@themad.hanbat.ac.kr  
? Direct SSH : ✓  
? SSH compression : ✓  
? SSH-browser : ✓  
? X11-forwarding : ✓ (remote display is forwarded through SSH)  
▶ For more info, ctrl+click on help or visit our website.
```

Welcome to Ubuntu 22.04.4 LTS (GNU/Linux 6.5.0-26-generic x86\_64)

\* Documentation: <https://help.ubuntu.com>  
\* Management: <https://landscape.canonical.com>  
\* Support: <https://ubuntu.com/pro>

Expanded Security Maintenance for Applications is not enabled.

57 updates can be applied immediately.  
To see these additional updates run: `apt list --upgradable`

3 additional security updates can be applied with ESM Apps.  
Learn more about enabling ESM Apps service at <https://ubuntu.com/esm>

\*\*\* System restart required \*\*\*  
Last login: Sun Apr 28 14:54:09 2024 from 210.110.251.150  
(base) team01@k10ud:~\$

Remote monitoring

Follow terminal folder

UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: <https://mobaxterm.mobatek.net>

파일이동

탐색기  
Drag and drop

터미널

OS: 리눅스

# Linux Command

- / : means directories
- ./ : present directories
- ../ : previous (one above) directories
- ~/ : home directories
- pwd = present working directory (현재위치)
- **ls = list** = showing the files and directories
  - ls (./)
  - ls ../
  - ls (./)name\_of\_directory/
- mkdir = make directory
  - mkdir (./)name\_of\_directory
  - mkdir ../name\_of\_directory
  - mkdir ../../name\_of\_directory
- **cd** = change directory
  - cd name\_of\_directory
  - cd ~/something/something/something/name\_of\_directory
- Linux doesn't allow 'space' (띄어쓰기 x)
- 영어이름이 기본
- Try to use 'tab' all the time (자동완성)
- 윗 화살표 (↑) : 직전사용한 명령어

기본적으로

‘[명령어] [주소]/[타겟]’ 의 형태

ex) cd ./test

ex) cd ~/something/something/test

ex) mkdir test

ex) mkdir ./test

ex) mkdir ~/something/something/test

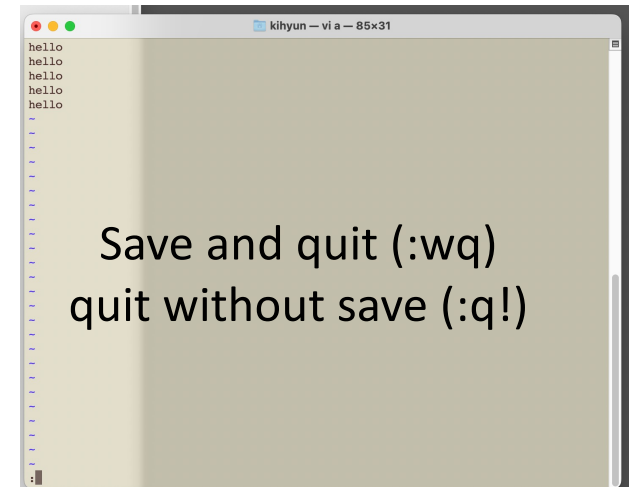
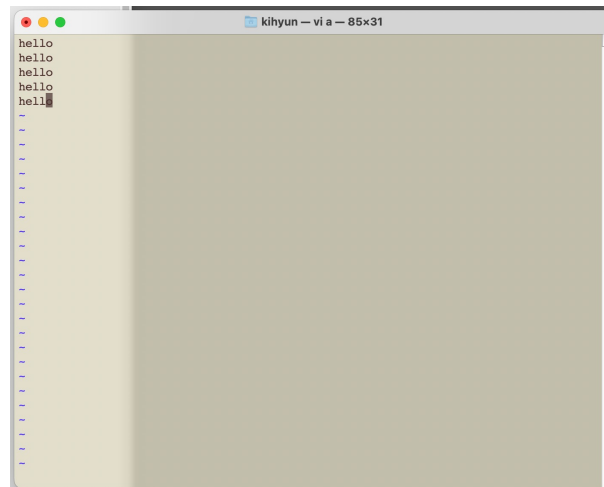
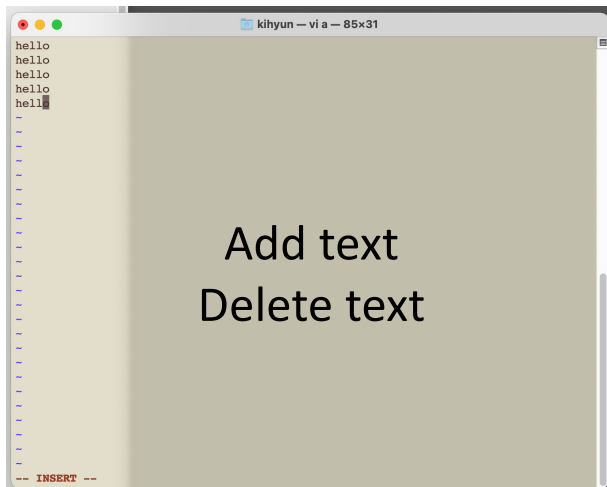
ex) cp ~/d/d/d/text ~/d/e/f/g

# Linux Command

- rmdir = remove directory (**only empty directory**)
  - rmdir name\_of\_directory
  - rmdir ../name\_of\_directory
- **rm** = remove files (**only files**)
  - rm name\_of\_files
  - **rm -rf name\_of\_directory\_or\_files : enforce the command**
- cp = copy files (or directory) to other directory
  - cp name\_of\_files ../name\_of\_directory
  - **cp test.txt example.txt : 복붙 이면서 파일이름 변경**
  - cp ../name\_of\_files ../name\_of\_directory
- mv = move files(or directory) to other directory (**오려두기 – 붙이기**)
  - Same as cp

# Linux Command

- vi editor = text editor
- vi = viewer
- Basic command : vi textfile
- If there is no file, will make file (열 파일이 없으면 생성)
- If there is file, will open file (열 파일이 있으면 오픈)



Three different modes

# XRD Simulation

## python xrd.py POSCAR\_FCC\_Cu

themad.hanbat.ac.kr (team01)

Terminal Sessions View X server Tools Games Settings Macros Help

Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help

Quick connect...

/home/team01/

Name

- ..
- .cache
- .conda
- .config
- miniconda3
- snap
- .bash\_history
- .bash\_logout
- .bashrc
- .profile
- .viminfo
- .Xauthority
- POSCAR\_FCC\_Cu
- xrd.png
- xrd.py

intensity

2θ

Remote monitoring

Follow terminal folder

```
? MobaXterm Personal Edition v24.1 ?
(SSH client, X server and network tools)

> SSH session to team01@themad.hanbat.ac.kr
? Direct SSH : ✓
? SSH compression : ✓
? SSH-browser : ✓
? X11-forwarding : ✓ (remote display is forwarded through SSH)

> For more info, ctrl+click on help or visit our website.

Welcome to Ubuntu 22.04.4 LTS (GNU/Linux 6.5.0-26-generic x86_64)

* Documentation: https://help.ubuntu.com
* Management: https://landscape.canonical.com
* Support: https://ubuntu.com/pro

Expanded Security Maintenance for Applications is not enabled.

57 updates can be applied immediately.
To see these additional updates run: apt list --upgradable

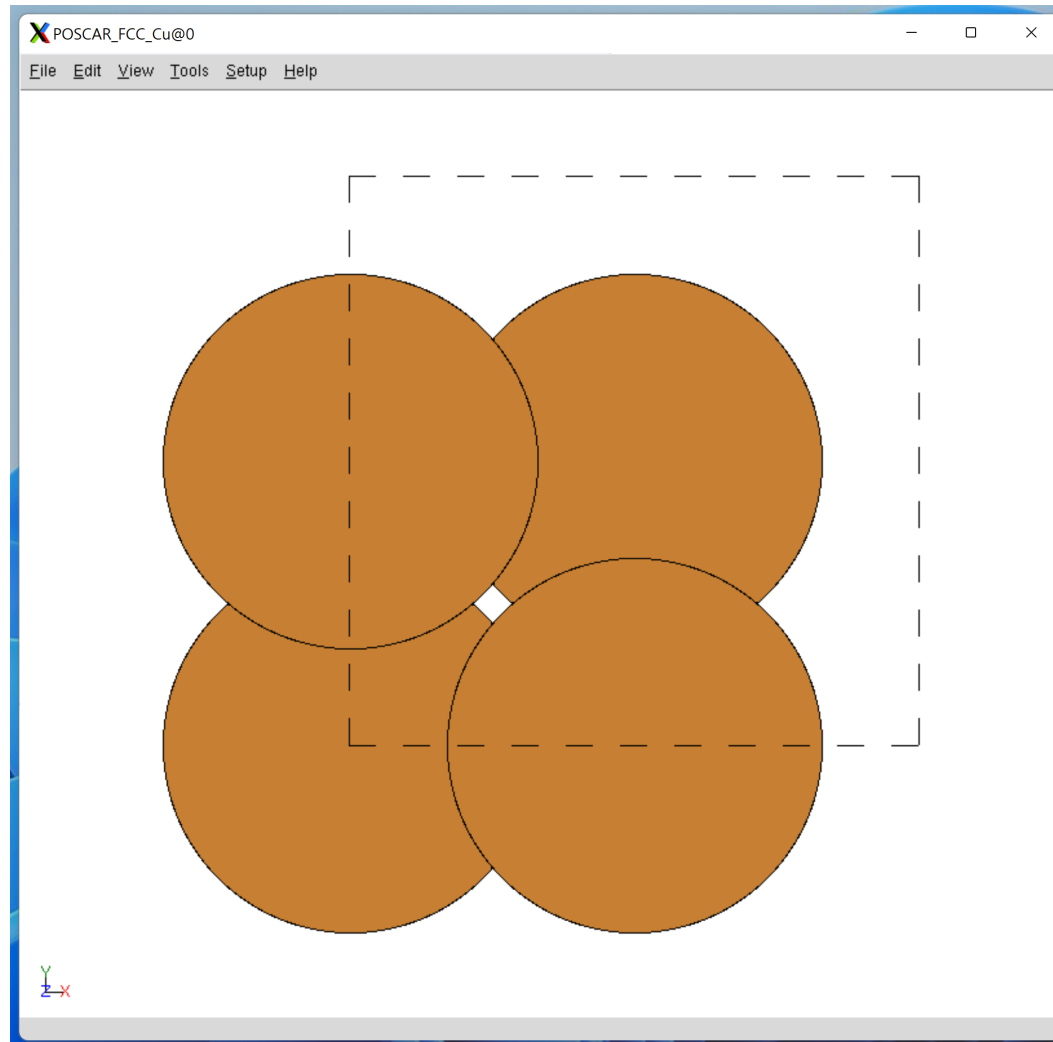
3 additional security updates can be applied with ESM Apps.
Learn more about enabling ESM Apps service at https://ubuntu.com/esm

*** System restart required ***
Last login: Sun Apr 28 14:56:35 2024 from 210.110.251.150
(base) team01@k10ud:~$ ls
miniconda3 POSCAR_FCC_Cu snap xrd.py
(base) team01@k10ud:~$ vi xrd.py
(base) team01@k10ud:~$ python xrd.py POSCAR_FCC_Cu
(base) team01@k10ud:~$ ls
miniconda3 POSCAR_FCC_Cu snap xrd.png xrd.py
(base) team01@k10ud:~$
```

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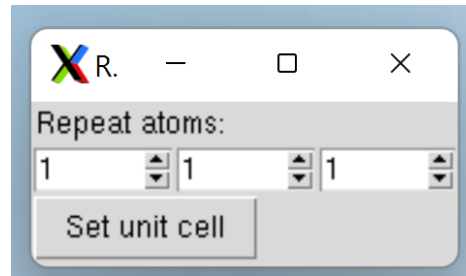
# XRD Simulation

**ase gui POSCAR\_FCC\_Cu**

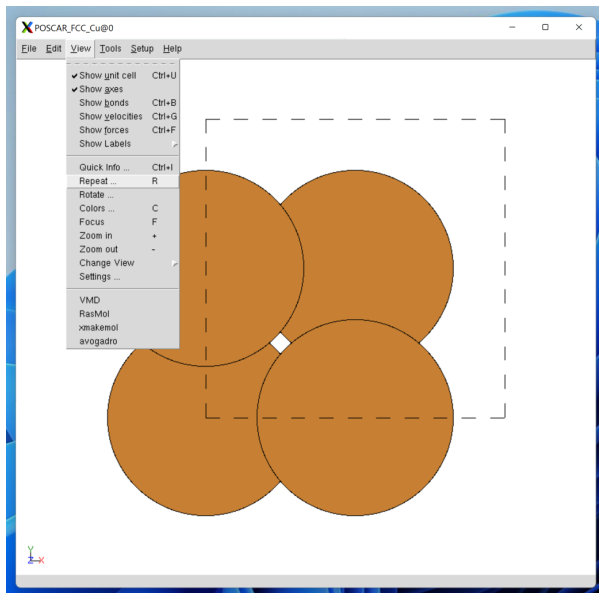


# XRD Simulation

**ase gui POSCAR\_FCC\_Cu**

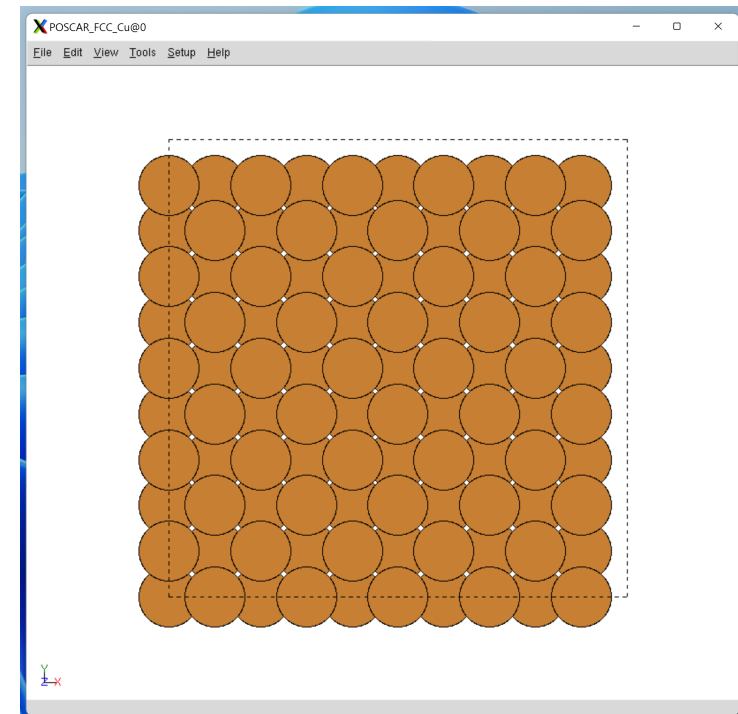


**다른이름으로 저장  
(POSCAR\_big)**



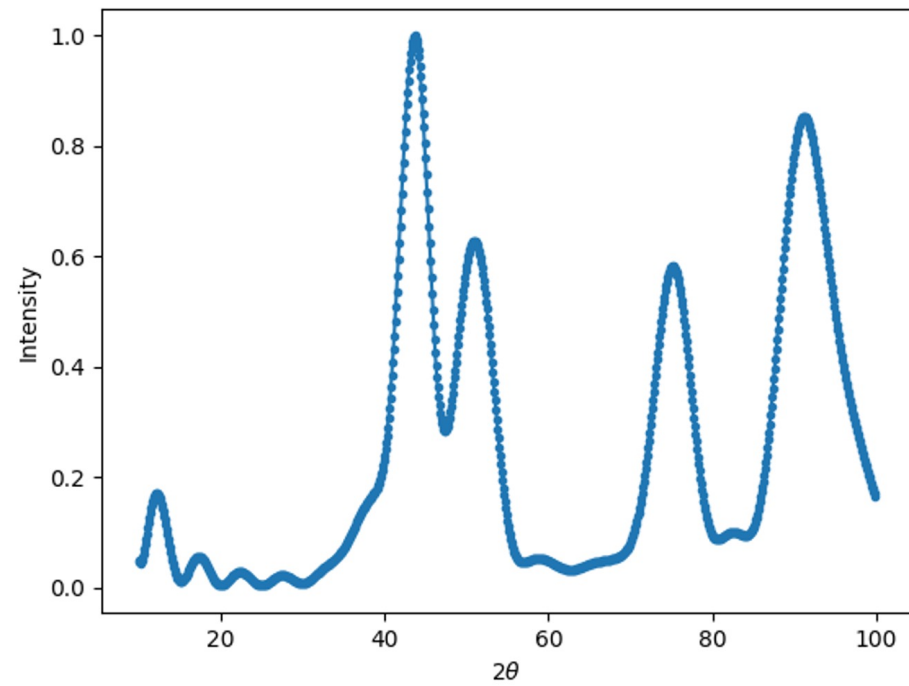
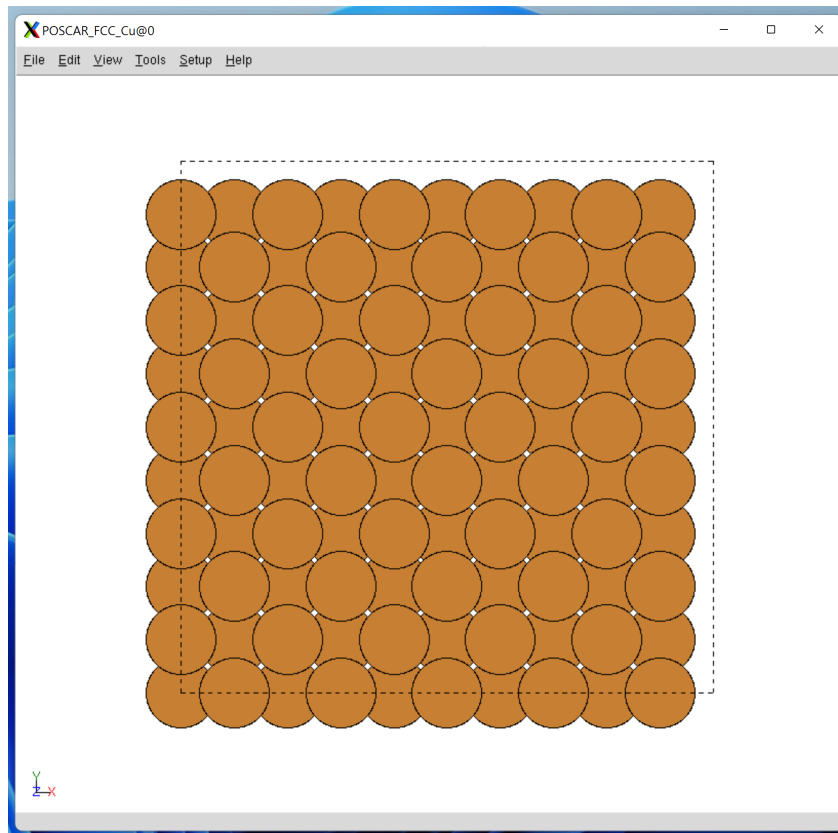
**숫자 키우고  
(5,5,5)**

**Set unit cell**



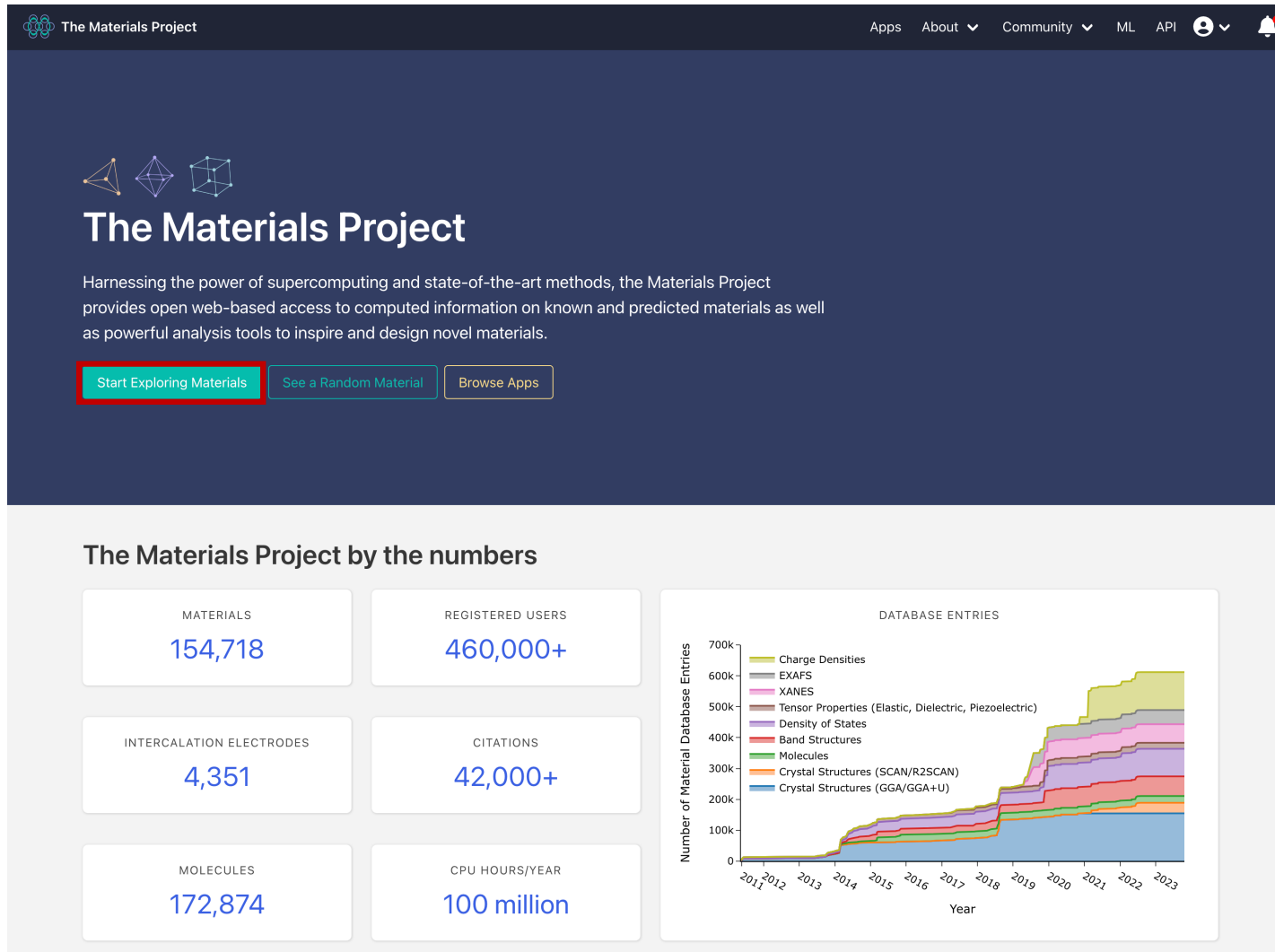
# XRD Simulation

**python xrd.py POSCAR\_big**



# How to get POSCAR file


Need to register ([next-gen.materialsproject.org](https://next-gen.materialsproject.org))




# How to get POSCAR file

Home / Apps / Materials Explorer

 Materials Explorer

 References

 Documentation

Search for materials information by chemistry, composition, or property.

Materials Cu



Search

Filters

Reset

▶ Composition 1 active

▶ Thermodynamics

▶ Structural Properties

▶ Symmetry

▶ Calculated Properties

▶ Electronic Structure

▶ Magnetism

▶ Elasticity

▶ Surfaces

▶ Piezoelectric


▶ Dielectric

8 materials match your search

Showing 1-8

✕ Chemical System: Cu

Columns ▾

 Export Table

Material ID	Formula	Crystal System	Space Group Symbol	Sites	Energy Above Hull (eV/atom)	Band Gap (eV)
<a href="#">mp-1010136</a>	Cu	Tetragonal	I4/mmm	1	0.04	0
★ <a href="#">mp-1056079</a>	Cu	Monoclinic	P12/m1	1	1.98	1.00
<a href="#">mp-1059259</a>	Cu	Orthorhombic	Cmcm	2	0.16	0
<a href="#">mp-1120774</a>	Cu	Trigonal	P3m1	6	0.18	0
★ <a href="#">mp-30</a>	Cu	Cubic	Fm3m	1	0	0
<a href="#">mp-989695</a>	Cu	Hexagonal	P6 <sub>3</sub> /mmc	4	< 0.01	0
<a href="#">mp-989782</a>	Cu	Hexagonal	P6 <sub>3</sub> /mmc	2	0.01	0
<a href="#">mp-998890</a>	Cu	Cubic	Im3m	1	0.03	0

Jump to ^

15 / page ^

← Previous


1


Next →

# How to get POSCAR file

Home / Apps / Materials Explorer / Cu / Cu / mp-30

 Materials Explorer

 References

 Documentati

**Cu**  
mp-30

TABLE OF CONTENTS

Summary

Crystal Structure

Properties

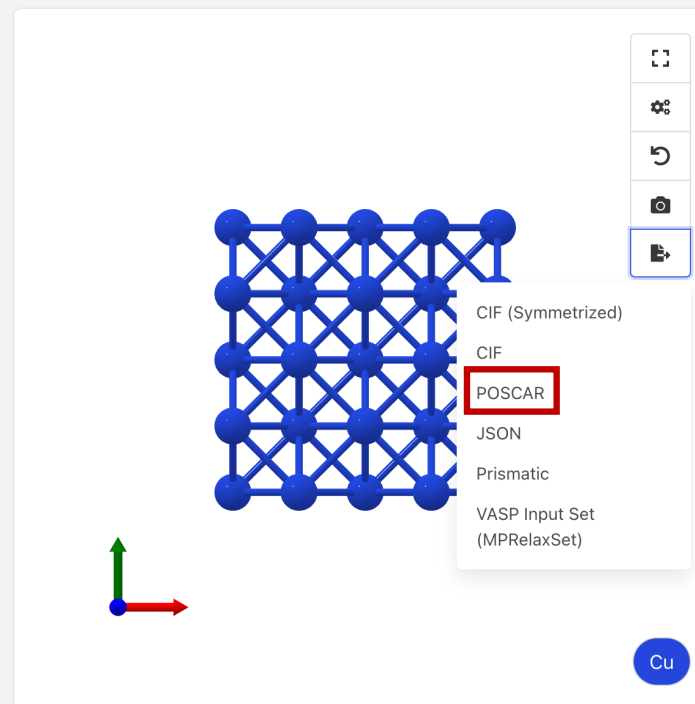
Contributed Data

Literature References

External Links

More

Related Materials



Energy Above Hull 0.000 eV/atom

Space Group  $Fm\bar{3}m$

Band Gap 0.00 eV

Predicted Formation Energy 0.000 eV/atom

Magnetic Ordering Non-magnetic

Total Magnetization 0.00  $\mu\text{B}/\text{f.u.}$

Experimentally Observed Yes

Description (Auto-generated)

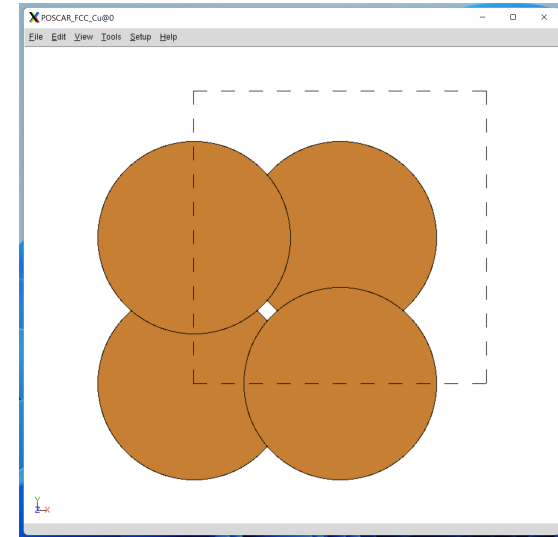
Cu is Copper structured and crystallizes in the cubic  $Fm\bar{3}m$  space group. Cu is bonded to twelve equivalent Cu atoms to form a mixture of edge, face, and corner-sharing  $\text{CuCu}_{12}$  cuboctahedra. All Cu-Cu bond lengths are 2.53 Å.

 Export Materials Details

# POSCAR

구조파일 (VASP이라는 프로그램에 사용하는)

POS (position) + CAR (fortran 에서 일반적으로 쓰는 파일명)



제목 (아무 의미 없음)

Cu4

Scaling factor (아래 박스 사이즈 조절)

1.0

3.5774306715697510 0.0000000000000000 0.0000000000000002 a 벡터

0.00000000000000006 3.5774306715697510 0.0000000000000002 b 벡터 박스 크기

0.00000000000000000 0.00000000000000000 3.5774306715697510 c 벡터

Cu 원소 종류

4 갯수

direct 좌표지정방법 (direct : 박스기준 분율, cartesian : 절대좌표)

0.00000000000000000 0.00000000000000000 0.00000000000000000 Cu

0.00000000000000000 0.50000000000000000 0.50000000000000000 Cu

0.50000000000000000 0.00000000000000000 0.50000000000000000 Cu

0.50000000000000000 0.50000000000000000 0.00000000000000000 Cu

각 원자들의 좌표

요건 없어도 무관

# POSCAR

**vi POSCAR\_big**

```
Cu
1.0000000000000000
 17.8871533578487565  0.0000000000000000
 0.000000000000000030 17.8871533578487565
 0.000000000000000000  0.0000000000000000
```

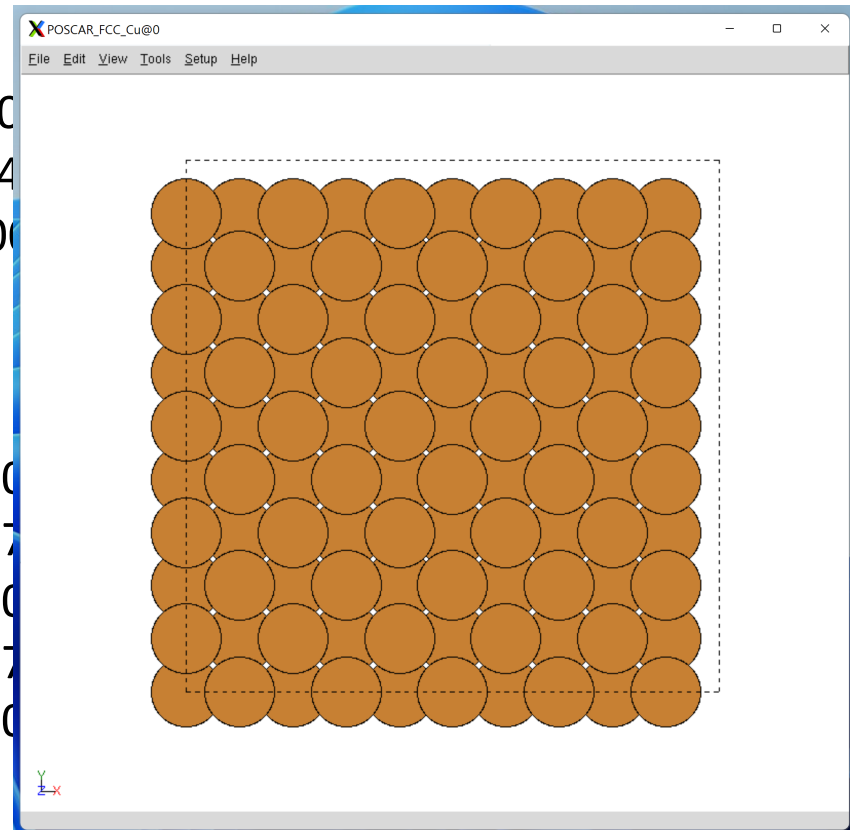
Cu

500

Cartesian

```
0.0000000000000000 0.0000000000000000
0.00000000000000003 1.7887153357848756
1.7887153357848755 0.0000000000000000
1.7887153357848757 1.7887153357848756
0.0000000000000000 0.0000000000000000
```

...



# Report and Presentation

**Sample: SC, BCC, FCC, HCP, Diamond, ???**

**1. Team01 (5/19)**

**방병조, 전진영, 최성민, 최은서, 민유빈**

**2. Team02 (5/19)**

**이찬복, 방현우, 남선미, 정소영, 박서연**

**3. Team03 (5/26)**

**임종범, 심태준, 오예원, 서지혜, 전영은**

**4. Team04 (5/26)**

**한준희, 명건우, 최현주, 길지수**

**'4개씩 XRD 그림제공'**

→ **XRD의 이론**

→ **각각이 어떤 구조인지**

→ **어떤 원소가 여기에 해당되는지**

→ **왜 Peak이 저렇게 나왔는지**

→ **추가 토의내용**

# Schedule

1	5월 12일	보고서/발표 작성 요령 + 이론	신기현
2	5월 19일	실습 (1조, 2조)	오장현
3	5월 26일	실습 (3조, 4조)	오장현
4	6월 2일	휴강	-
5	6월 9일	발표평가	신기현

**XRD Simulation** : 오장현 조교에게 문의 ()

강의자료 및 상세내용들은 홈페이지 참고 ([themad.hanbat.ac.kr](http://themad.hanbat.ac.kr))

# Evaluation

## 1. 보고서는 **개인** 제출 - 6/16일 까지 (이후 제출 0점)

- 양식 (양식은 홈페이지 참고) 미활용시 감점 (-5)
- 팀원끼리는 토의만 진행 → 보고서 내용이 동일할 경우 모두 0점
- 보고서의 포맷 및 퀄리티 (예쁘게 깔끔하게) 가 좋을 경우 가산점 (+5) 반대의 경우 (-5)
- 보고서 표지 만들 것 (+5)

## 2. 발표는 **팀별로 (10분 분량 준비)** - 6/9일

- 발표자에게는 가산점 (단, 발표내용을 적어서 읽을 경우 가산점 X) (+5)
- 발표자료의 포맷 및 퀄리티 (예쁘게, 깔끔하게) 가 좋을 경우 가산점 (+5) 반대의 경우 (-5)
- 발표태도가 뛰어나면 가산점 (+3)
- 질문을 할 경우에 가산점 (+5)

# One more thing ...

**모두가 생성형 AI 를 사용한다.**

**어떻게 해야 좋은 평가를 받을 수 있나?**

**→ 나만의 창의적, 차별적 접근법 필요**