

2024년도 1학기 신소재공학실험(1)

신기현 (조교: 도연우)

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Schedule

9	4월 30일	보고서/발표 작성 요령 + 이론	신기현
10	5월 7일	team01 (XRD Simulation)	도연우
11	5월 14일	team02 (XRD Simulation)	도연우
12	5월 21일	team03 (XRD Simulation)	도연우
13	5월 28일	team04 (XRD Simulation)	도연우
14	6월 4일	발표평가	신기현
15	6월 11일	기말고사	X

XRD Simulation : 도연우 조교님에게 문의 (20211522@edu.hanbat.ac.kr)

강의자료 및 상세내용들은 홈페이지 참고 (themad.hanbat.ac.kr)

Team

1. team01

박준영, 박진우, 김민하, 문채원, 권준길, 금대호

2. team02

천재호, 박종민, 김영재, 명승주, 김태훈, 김민아

3. team03

정인성, 임태경, 주한울, 김지환, 유지희, 박시룡

4. team04

오성연, 황규빈, 권도익, 윤소연, 전소희, 윤건영, 김현

Evaluation

1. 보고서는 **개인** 제출 - 6/18일 까지 (이후 제출 0점)

- 조교님에게 PDF로 제출 (-5)
- 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)** - 6/4일

- 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”)

독배기 보다 장맛이 좋다
(먹어봐야 안다)

Fundamentals of XRD

X선 회절 = XRD (**X-ray** Diffraction)

X-ray wavelength : 0.01 ~ 10 nm

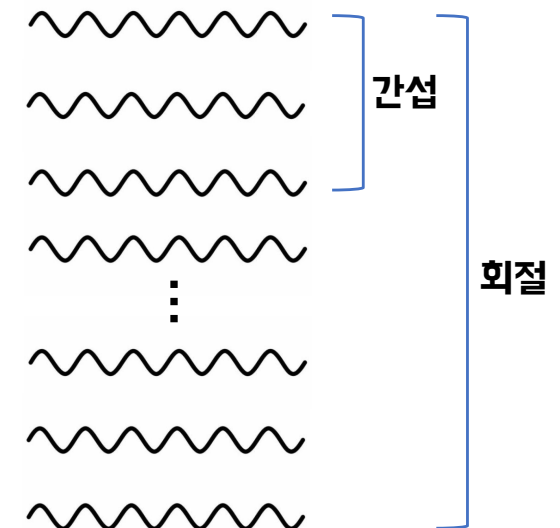
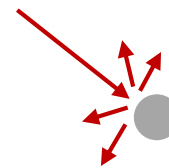
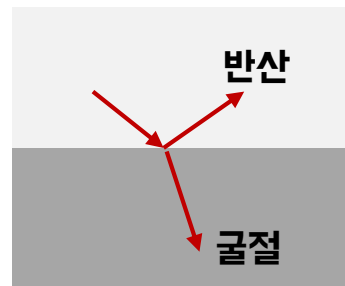
Scale of atom : 1 Å = 0.1 nm

$\text{CuK}\alpha = 1.5406 \text{ \AA}$

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.

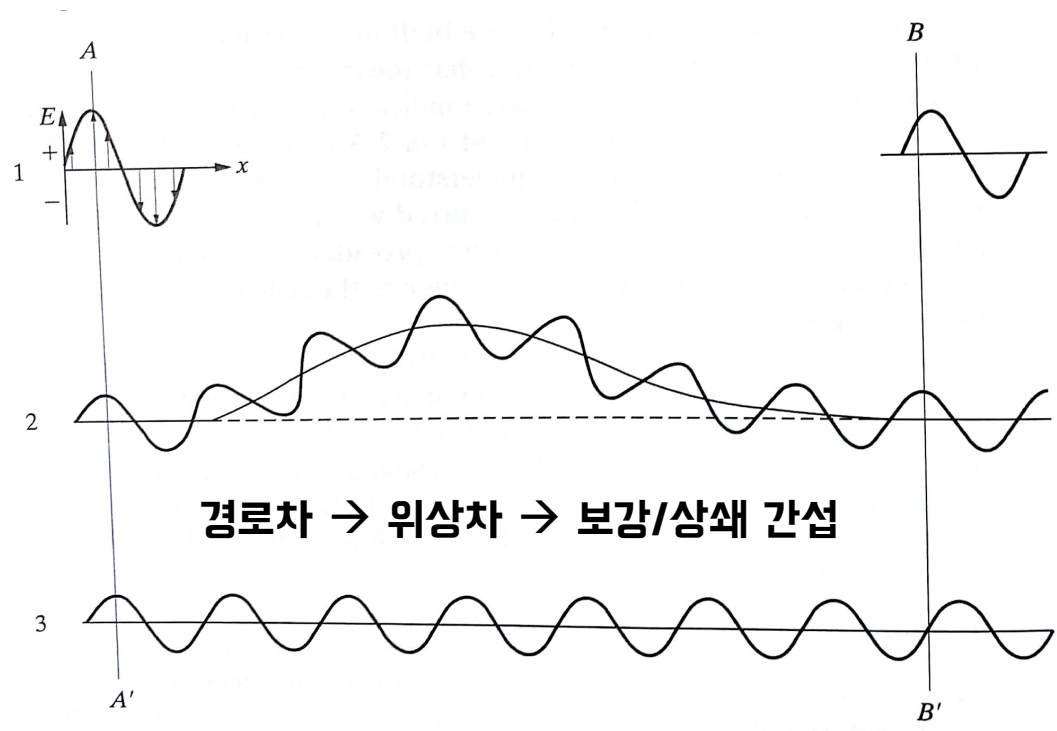
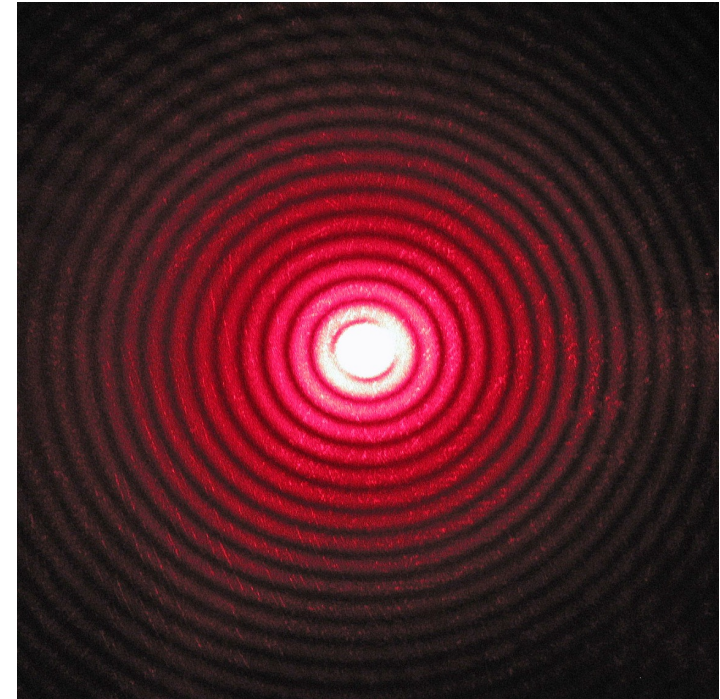
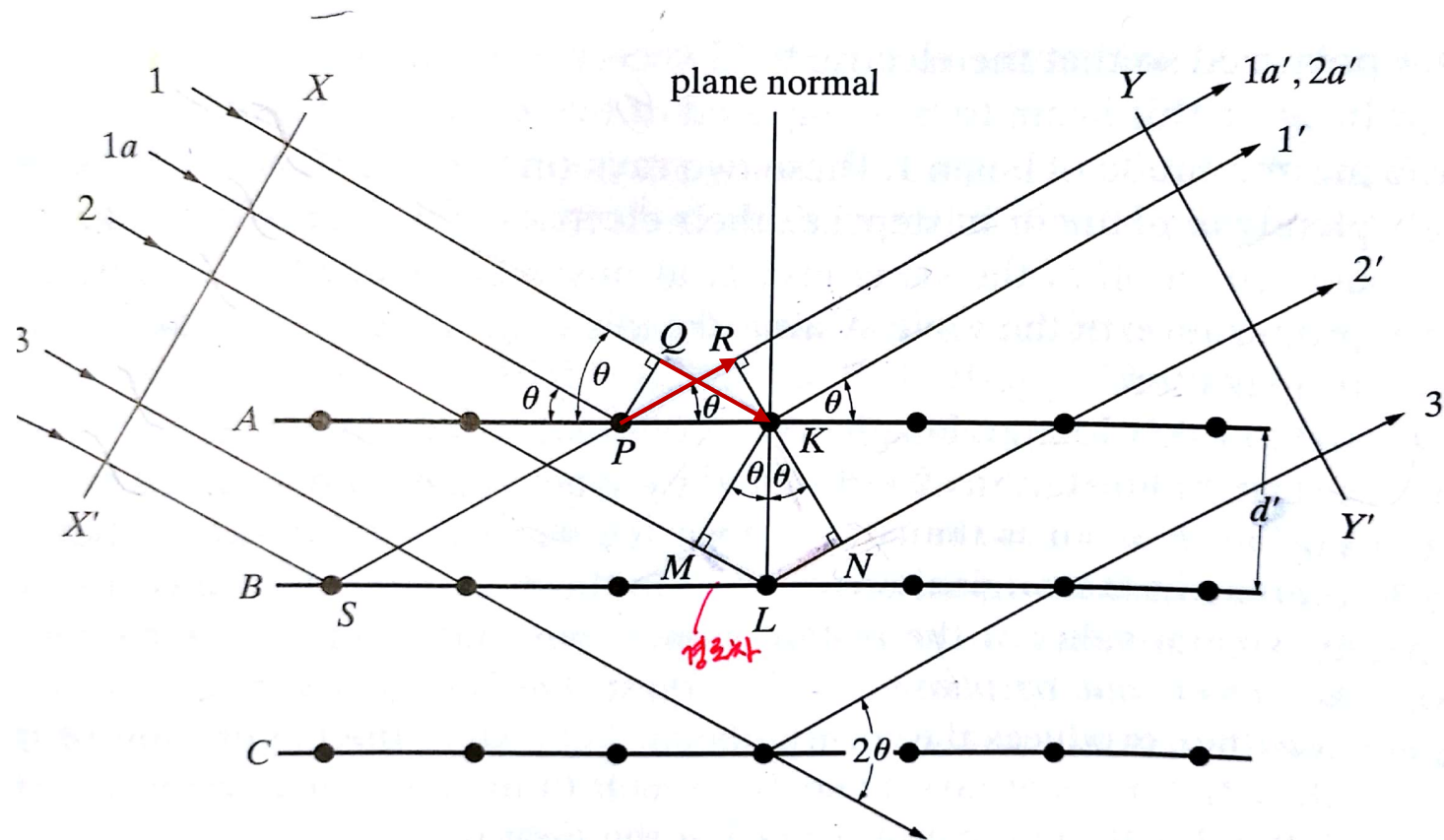


Figure 3-1 Effect of path difference on relative phase.

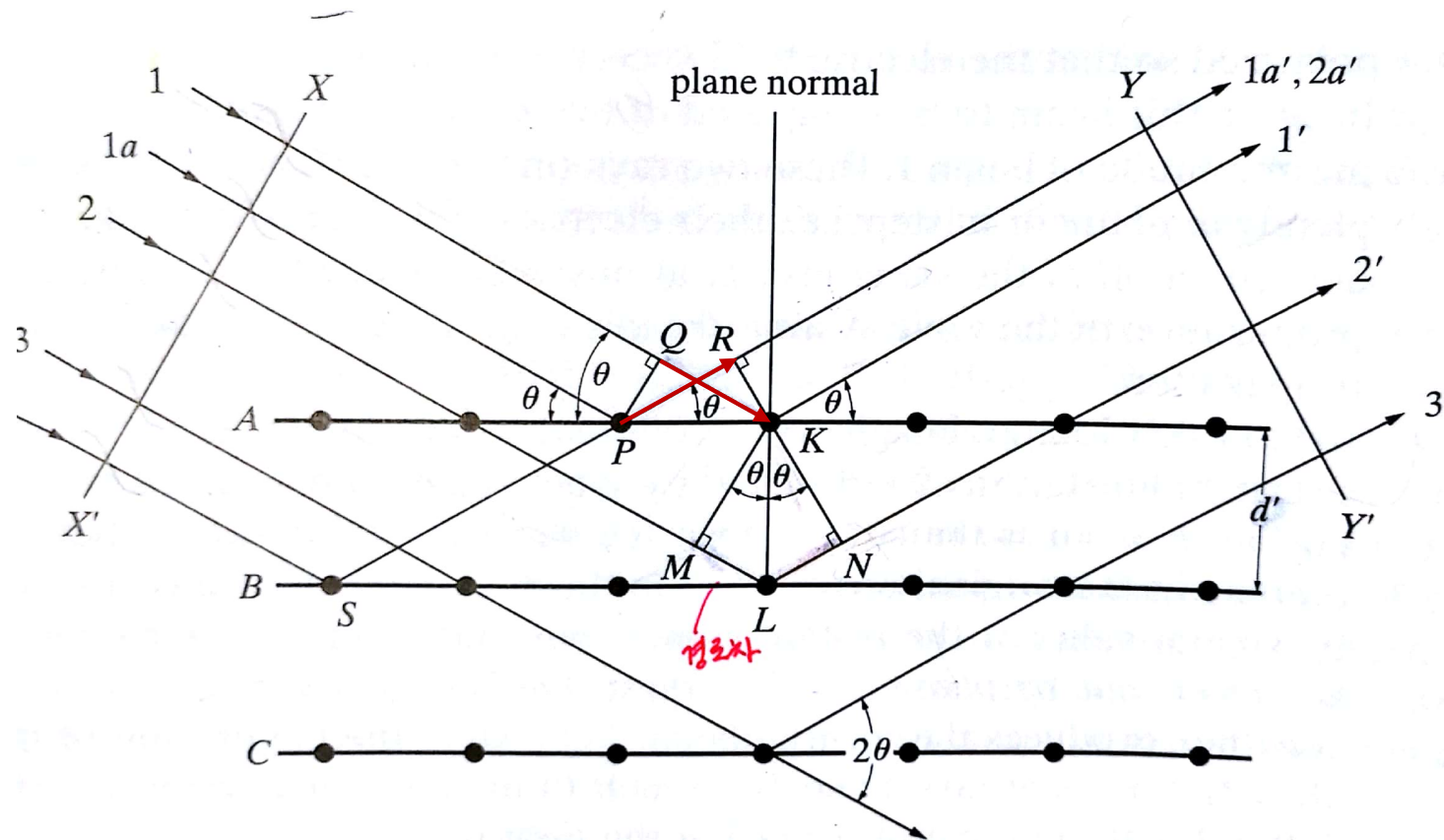


Bragg's Law



조건 : 면간거리 d' 의 결정. 파장 λ 의 X-ray 가 θ 각으로 조사되었을 때

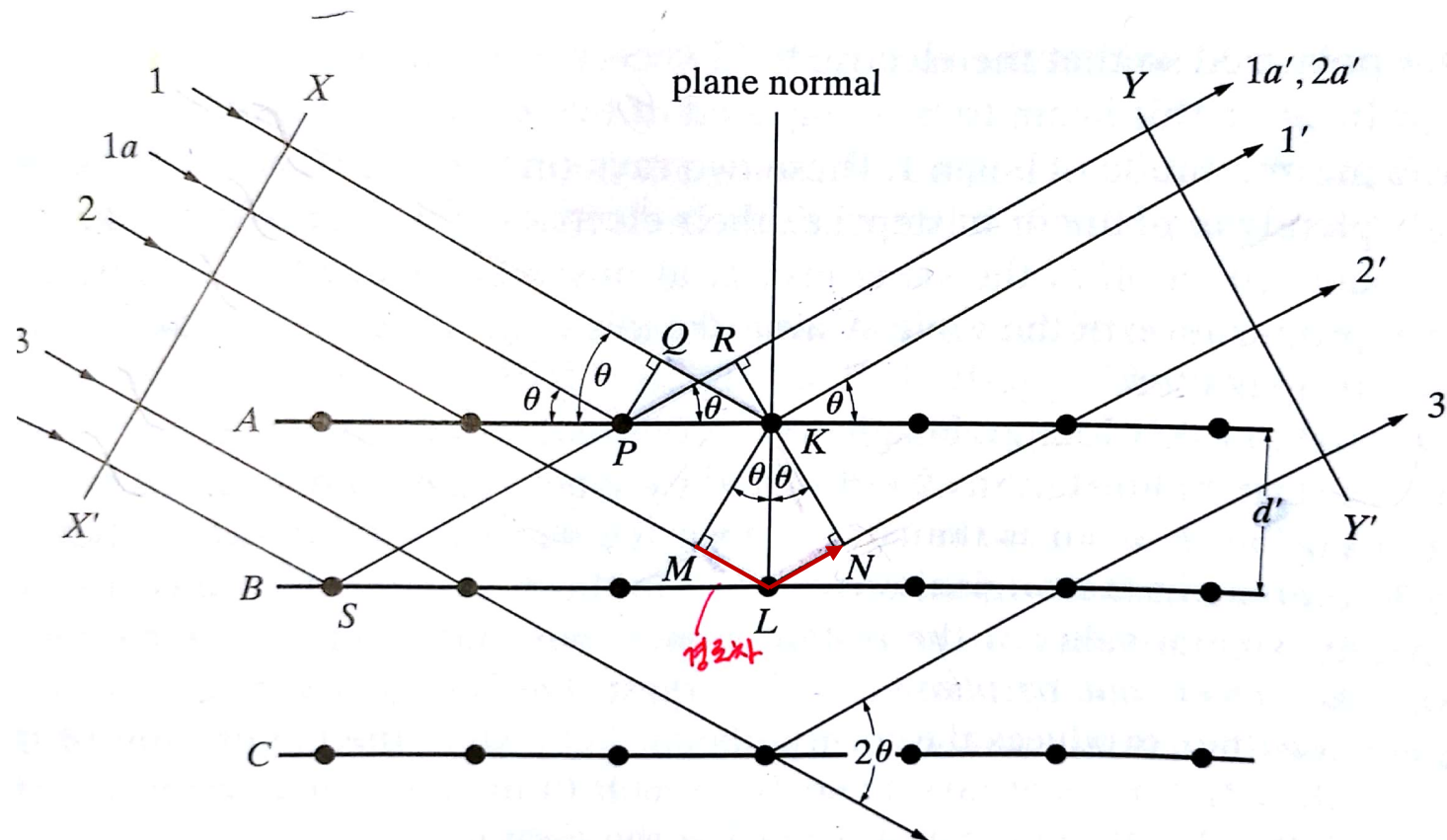
Bragg's Law



1. 같은 면에서 입사각과 산란각이 같을 때 회절 (1-1', 1a-1a'의 경우)

$$QK - PR (\text{경로차}) = PK \cos \theta - PK \cos \theta = 0 \rightarrow \text{경로 차가 없다. in phase}$$

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 → 1st order 사용

Diffraction Direction

결정격자별 (hkl) 면의 peak 의 위치 (θ)

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

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

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		
He	2	1.88	1.46	1.05	0.75	0.52	0.35	0.24	0.18	0.14	0.11	0.09		
Li ⁺	2	1.96	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4	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		
Be ⁺²	2	2.0	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7	0.6	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		
B ⁺³	2	1.99	1.9	1.8	1.7	1.6	1.4	1.3	1.2	1.0	0.9	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		
C	6	4.6	3.0	2.2	1.9	1.7	1.6	1.4	1.3	1.16	1.0	0.9		
N ⁺⁵	2	2.0	2.0	1.9	1.9	1.8	1.7	1.6	1.5	1.4	1.3	1.16		
N ⁺³	4	3.7	3.0	2.4	2.0	1.8	1.66	1.56	1.49	1.39	1.28	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		
O	8	7.1	5.3	3.9	2.9	2.2	1.8	1.6	1.5	1.4	1.35	1.26		
O ⁻²	10	8.0	5.5	3.8	2.7	2.1	1.8	1.5	1.5	1.4	1.35	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		
F ⁻	10	8.7	6.7	4.8	3.5	2.8	2.2	1.9	1.7	1.55	1.5	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		
Na ⁺	10	9.5	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95	1.75	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		
Mg ⁺²	10	9.75	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2	2.0	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		
Al ⁺³	10	9.7	8.9	7.8	6.65	5.5	4.45	3.65	3.1	2.65	2.3	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		
Si ⁺⁴	10	9.75	9.15	8.25	7.15	6.05	5.05	4.2	3.4	2.95	2.6	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		
P ⁺⁵	10	9.8	9.25	8.45	7.5	6.55	5.65	4.8	4.05	3.4	3.0	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		
P ⁻³	18	12.7	9.8	8.4	7.45	6.5	5.65	4.85	4.05	3.4	3.0	2.6		
S ⁺⁶	10	9.85	9.4	8.7	7.85	6.85	6.05	5.25	4.5	3.9	3.35	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		
S ⁻²	18	14.3	10.7	8.9	7.85	6.85	6.0	5.25	4.5	3.9	3.35	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		
Cl ⁻	18	15.2	11.5	9.3	8.05	7.25	6.5	5.75	5.05	4.4	3.85	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		
K ⁺	18	16.5	13.3	10.8	8.85	7.75	7.05	6.44	5.9	5.3	4.8	4.2		
K	19	16.5	13.3	10.8	9.2	7.9	7.1	6.4	5.9	5.2	4.6	4.2	3.7	3.3
Ca ⁺²	18	16.8	14.0	11.5	9.3	8.1	7.35	6.7	6.2	5.7	5.1	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	
Sc ⁺³	18	16.7	14.0	11.4	9.4	8.3	7.6	6.9	6.4	5.8	5.35	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	
Ti ⁺⁴	18	17.0	14.4	11.9	9.9	8.5	7.85	7.3	6.7	6.15	5.65	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	
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	
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	
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	

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.

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Connecting Server

The screenshot displays the MobaXterm application window. The main area shows connection details: Host: themad.hanbat.ac.kr, Username: team01 ~ team 04, and PW: n8318. A 'Session settings' dialog box is open, with the 'SSH' option selected in the top toolbar. The 'Basic SSH settings' section is highlighted, showing 'Remote host * themad.hanbat.ac.kr', 'Specify username' checked with 'team01' in the dropdown, and 'Port 22'. The 'Advanced SSH settings' section includes 'X11-Forwarding' and 'Compression' checked, 'Remote environment' set to 'Interactive shell', 'Execute command' field, 'SSH-browser type' set to 'SFTP protocol', and 'Use private key' unchecked. 'Execute macro at session start' is set to '<none>'. 'OK' and 'Cancel' buttons are at the bottom.

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

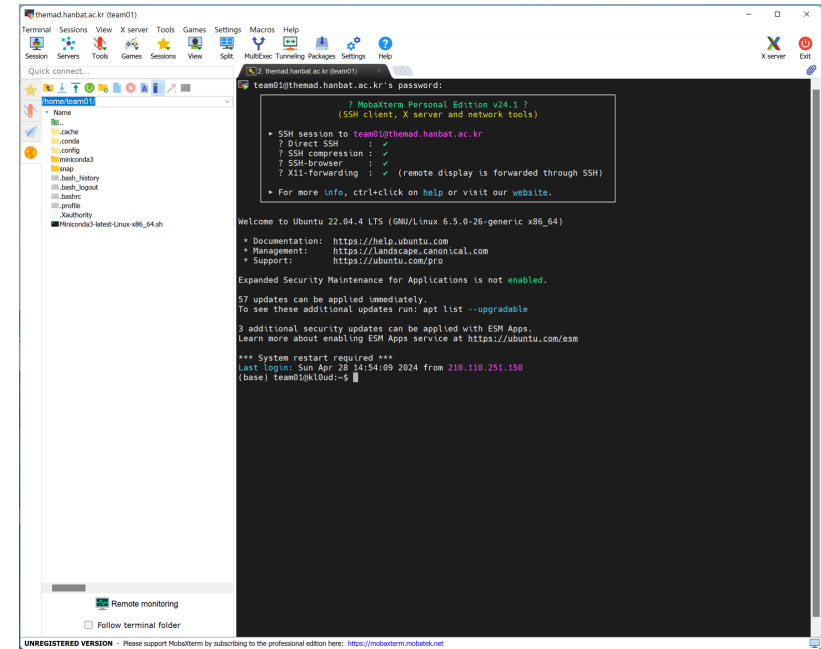
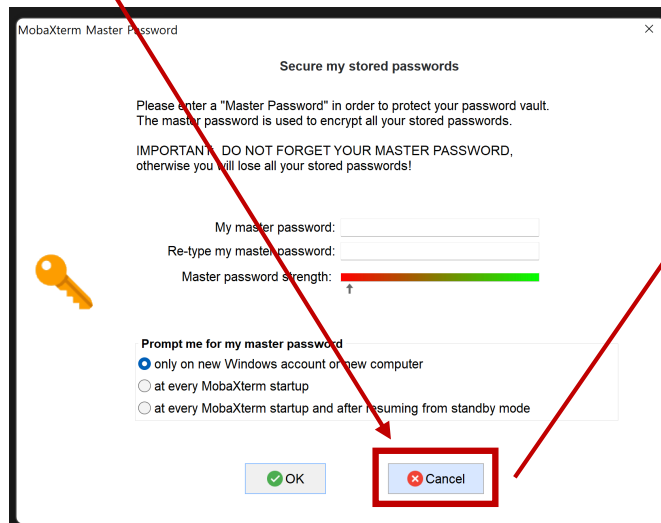
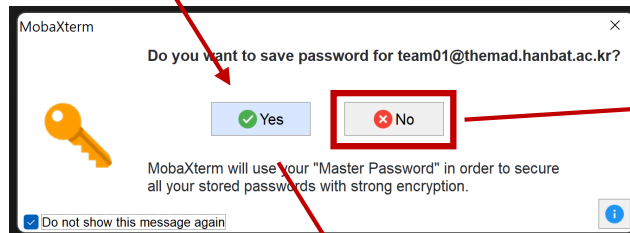
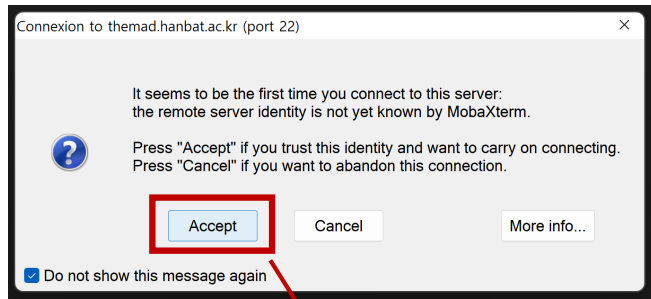
SSH-browser type: SFTP protocol Follow SSH path (experimental)

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

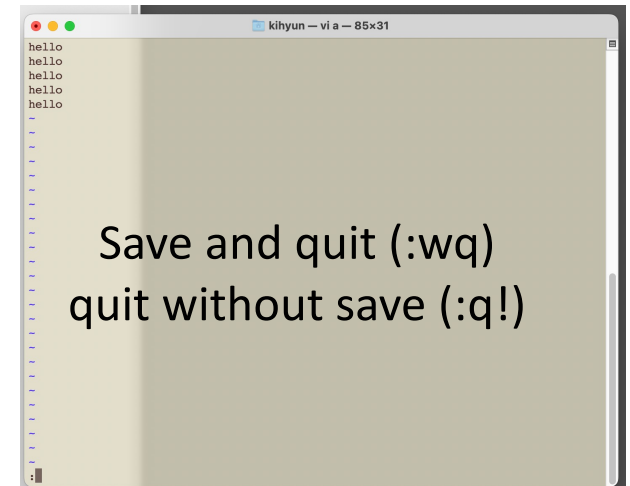
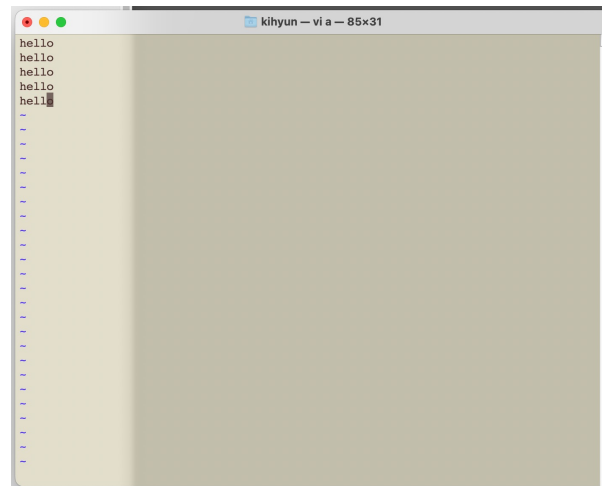
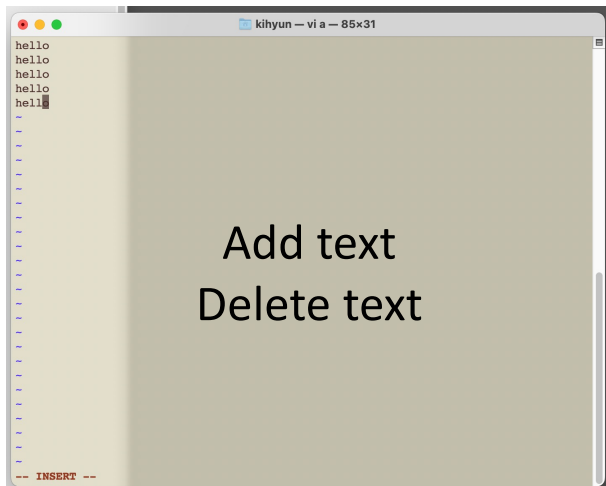
ex) cp ~/d/d/d/text ~/d/e/f/g

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

The screenshot shows a MobaXterm terminal window with a file explorer on the left. The file explorer displays the directory `/home/team01/` with files `xrd.png` and `xrd.py`. A red arrow points from `xrd.png` to a plot of Intensity vs. 2θ. The plot shows a sharp peak at approximately 20° 2θ and a broader peak at approximately 45° 2θ. The terminal window displays the following output:

```
? 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.

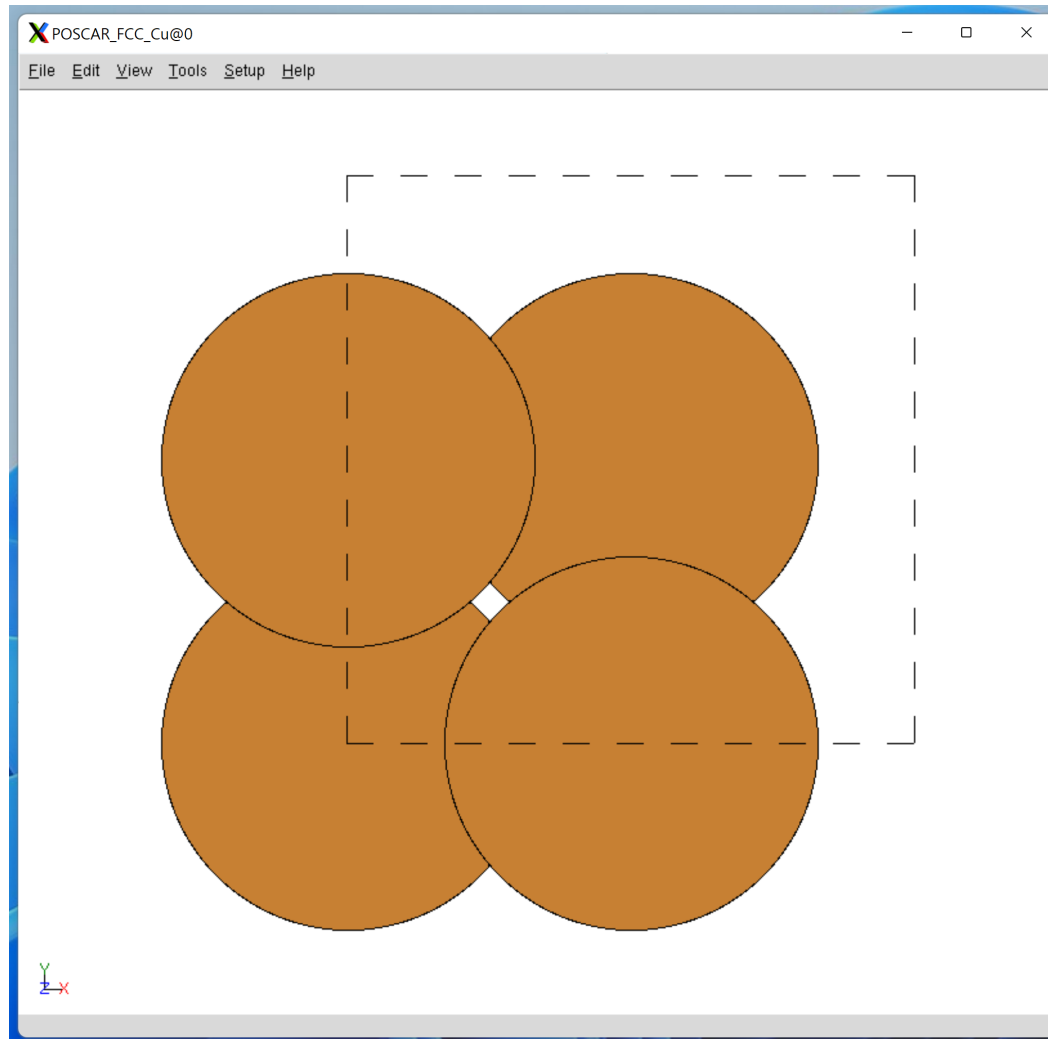
57 updates can be applied immediately.
To see these additional updates run: apt list --upgradable

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:~$
```

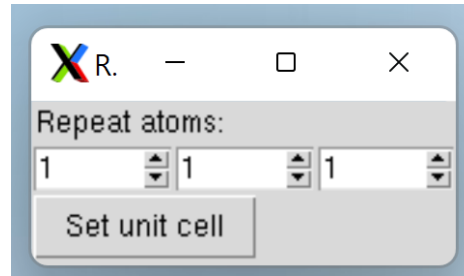

XRD Simulation

ase gui POSCAR_FCC_Cu

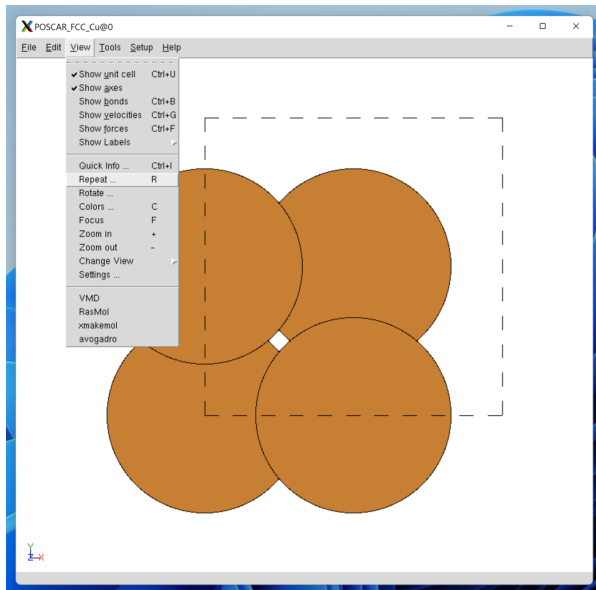


XRD Simulation

ase gui POSCAR_FCC_Cu

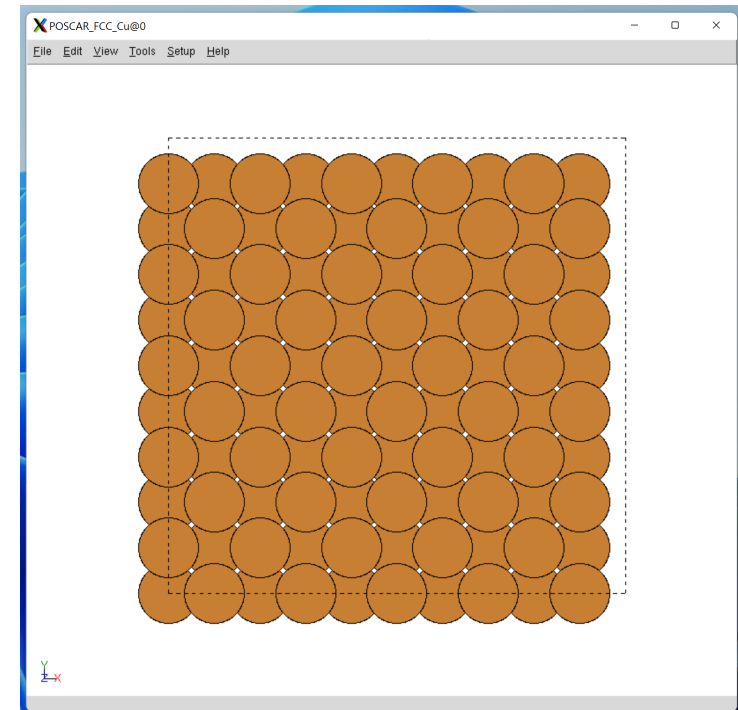


다른이름으로 저장
(POSCAR_big)



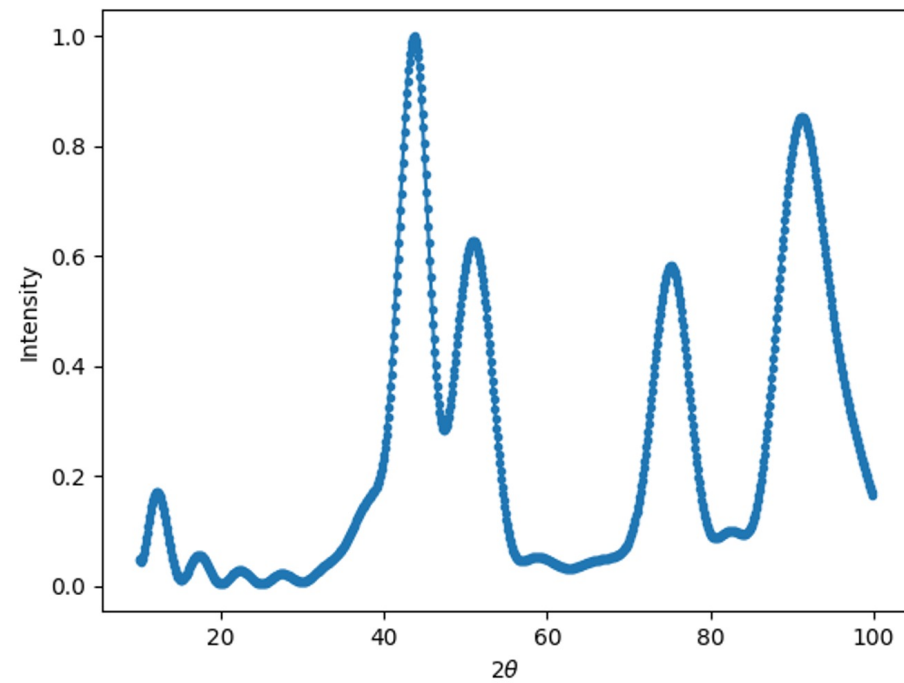
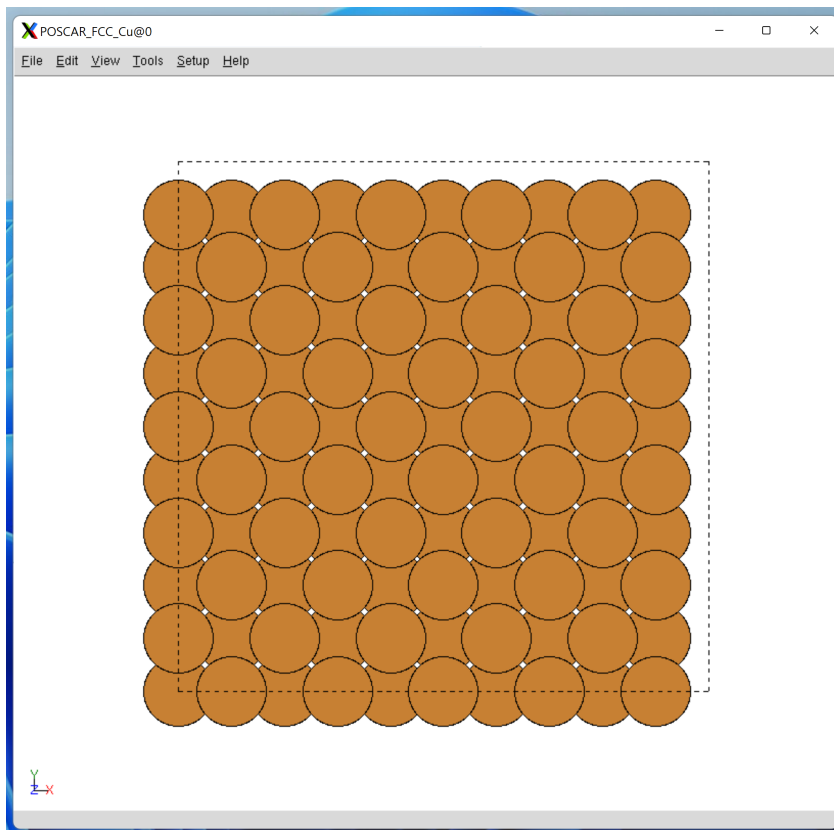
숫자 키우고
(5,5,5)

Set unit cell



XRD Simulation

python xrd.py POSCAR_big



How to get POSCAR file

Need to register (next-gen.materialsproject.org)

The screenshot shows the homepage of The Materials Project. At the top, there is a navigation bar with links for 'Apps', 'About', 'Community', 'ML', 'API', and user profile/notification icons. The main header features the project logo and the title 'The Materials Project'. Below the title, a short description states: 'Harnessing the power of supercomputing and state-of-the-art methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.' Three buttons are visible: 'Start Exploring Materials' (highlighted with a red border), 'See a Random Material', and 'Browse Apps'.

The Materials Project by the numbers

MATERIALS	REGISTERED USERS
154,718	460,000+
INTERCALATION ELECTRODES	CITATIONS
4,351	42,000+
MOLECULES	CPU HOURS/YEAR
172,874	100 million

DATABASE ENTRIES

Legend for Database Entries:

- Charge Densities
- EXAFS
- XANES
- Tensor Properties (Elastic, Dielectric, Piezoelectric)
- Density of States
- Band Structures
- Molecules
- Crystal Structures (SCAN/R2SCAN)
- Crystal Structures (GGA/GGA+U)

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)
mp-1010136	Cu	Tetragonal	I4/mmm	1	0.04	0
★ mp-1056079	Cu	Monoclinic	P12/m1	1	1.98	1.00
mp-1059259	Cu	Orthorhombic	Cmcm	2	0.16	0
mp-1120774	Cu	Trigonal	P3m1	6	0.18	0
★ mp-30	Cu	Cubic	Fm3m	1	0	0
mp-989695	Cu	Hexagonal	P6 ₃ /mmc	4	< 0.01	0
mp-989782	Cu	Hexagonal	P6 ₃ /mmc	2	0.01	0
mp-998890	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

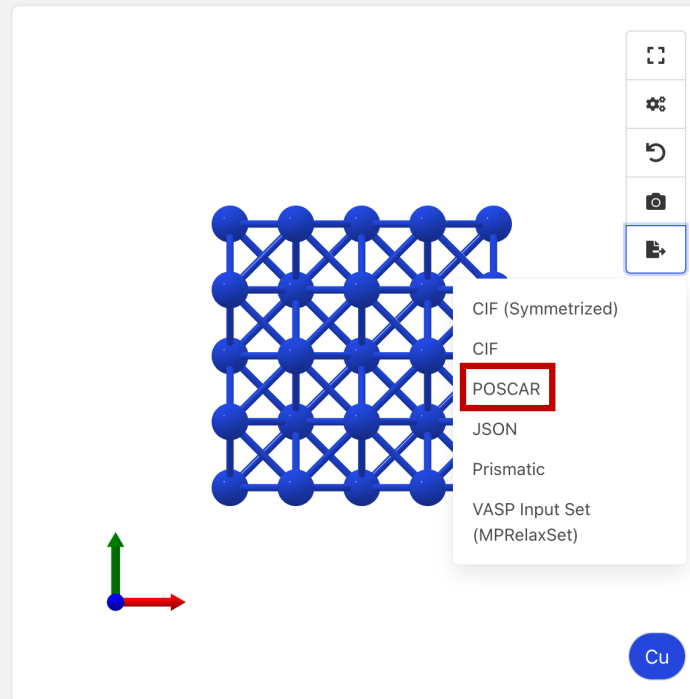
Contributed Data

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)

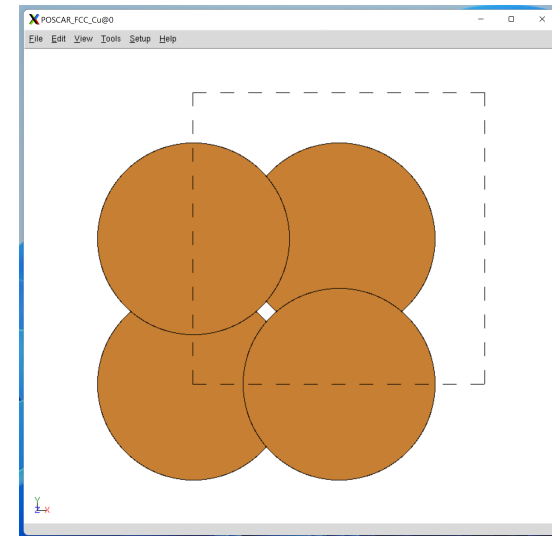
Cu is Copper structured and crystallizes in the cubic $Fm\bar{3}m$ space group. Cu is bonded to twelve equivalent Cu atoms to form a mixture of edge, face, and corner-sharing CuCu_{12} cuboctahedra. All Cu-Cu bond lengths are 2.53 Å.

 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	박스 크기
0.0000000000000006	3.5774306715697510	0.0000000000000002	b 벡터	
0.0000000000000000	0.0000000000000000	3.5774306715697510	c 벡터	

Cu → 원소 종류

4 → 갯수

direct → 좌표지정방법 (direct : 박스기분 분율, cartesian : 절대좌표)

0.0000000000000000	0.0000000000000000	0.0000000000000000	Cu	각 원자들의 좌표
0.0000000000000000	0.5000000000000000	0.5000000000000000	Cu	
0.5000000000000000	0.0000000000000000	0.5000000000000000	Cu	
0.5000000000000000	0.5000000000000000	0.0000000000000000	Cu	

요건 없어도 무관

POSCAR

vi POSCAR_big

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

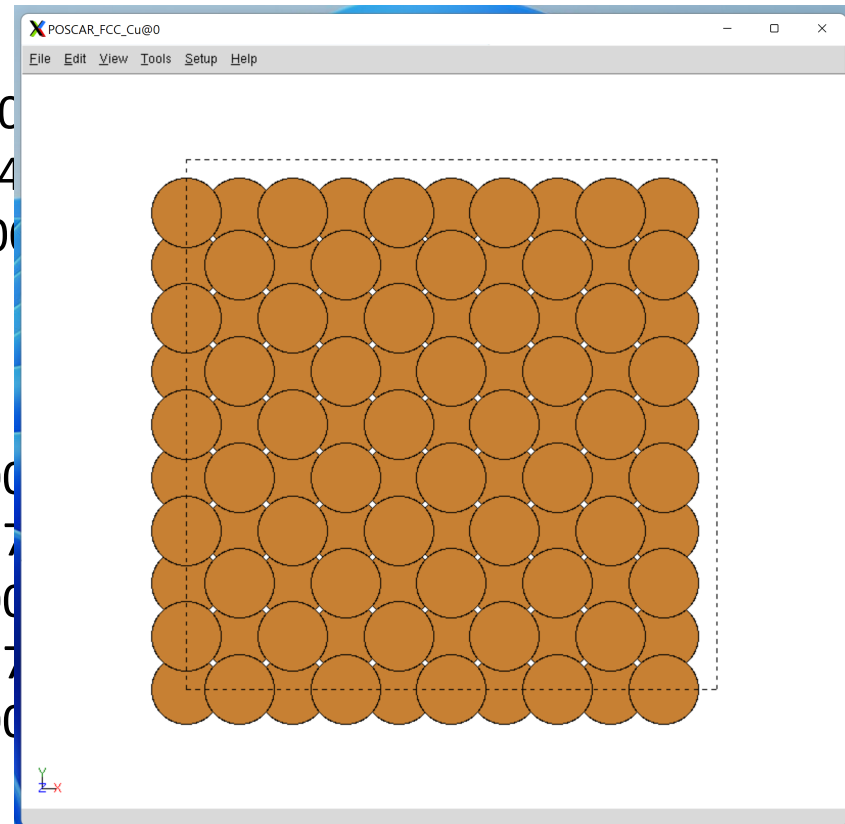
Cu

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

박준영, 박진우, 김민하, 문채원, 권준길, 금대호

2. team02

천재호, 박종민, 김영재, 명승주, 김태훈, 김민아

3. team03

정인성, 임태경, 주한울, 김지환, 유지희, 박시룡

4. team04

오성연, 황규빈, 권도익, 윤소연, 전소희, 윤건영, 김현

'4개씩 XRD 그림제공'

→ XRD의 이론

→ 각각이 어떤 구조인지

→ 어떤 원소가 여기에 해당되는지

→ 왜 Peak이 저렇게 나왔는지

→ 기타 등등...

→ 토의내용

Schedule

9	4월 30일	보고서/발표 작성 요령 + 이론	신기현
10	5월 7일	team01 (XRD Simulation)	도연우
11	5월 14일	team02 (XRD Simulation)	도연우
12	5월 21일	team03 (XRD Simulation)	도연우
13	5월 28일	team04 (XRD Simulation)	도연우
14	6월 4일	발표평가	신기현
15	6월 11일	기말고사	X

XRD Simulation : 도연우 조교님에게 문의 (20211522@edu.hanbat.ac.kr)

강의자료 및 상세내용들은 홈페이지 참고 (themad.hanbat.ac.kr)

Evaluation

1. 보고서는 **개인** 제출 - 6/18일 까지 (이후 제출 0점)

- 조교님에게 PDF로 제출 (-5)
- 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)** - 6/4일

- 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)