It's cute (可愛)……

But does it DO anything??

Powder diffraction - applications

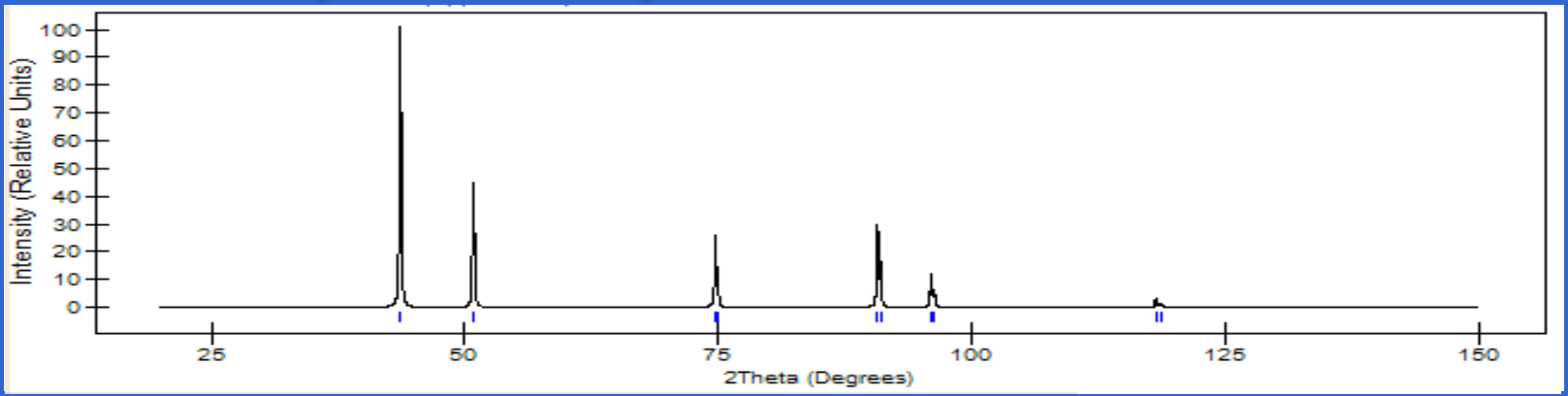
Qualitative analysis - what IS this stuff?!!

Every material has a unique x-ray powder pattern
Every PHASE has a unique powder pattern

This image, taken under a microscope, shows that a 'duplex stainless steel' has two phases

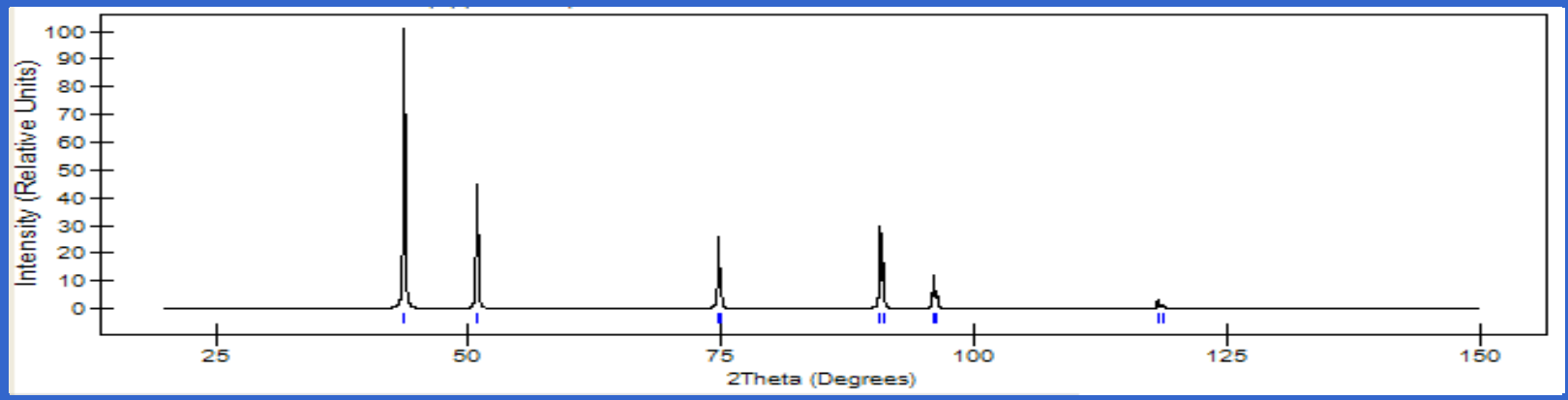
双相不锈钢

This is the X-ray diffraction pattern



Powder diffraction - applications

Qualitative analysis - what IS this stuff?!!



The X-ray diffraction pattern tells us this

How?

Powder diffraction - applications

Qualitative analysis - what IS this stuff?!!

We use the Powder Diffraction File database (the PDF)
and a search system

History

1938 Hanawalt paper on first database and search method
1941 ASTM committee publishes database on cards
1969 JCPDS incorporated; publishes the JCPDF

Powder diffraction - applications

Qualitative analysis - what IS this stuff?!!

We use the Powder Diffraction File database (the PDF)
and a search system

History

1938 Hanawalt paper on first database and search method
1941 ASTM committee publishes database on cards
1969 JCPDS incorporated; publishes the JCPDF
1977 JCPDS became the International Centre for Diffraction Data (ICDD) - currently publishing various databases, including the new PDF-4, with diffraction and structure data for >300,000 phases

PDF Card - Ca Cu - 04-007-1562

File Edit d-Spacings Tools Window Help

d-Spacings

Wavelength

Cu Kα1 1.54056Å

Å

Stick Pattern

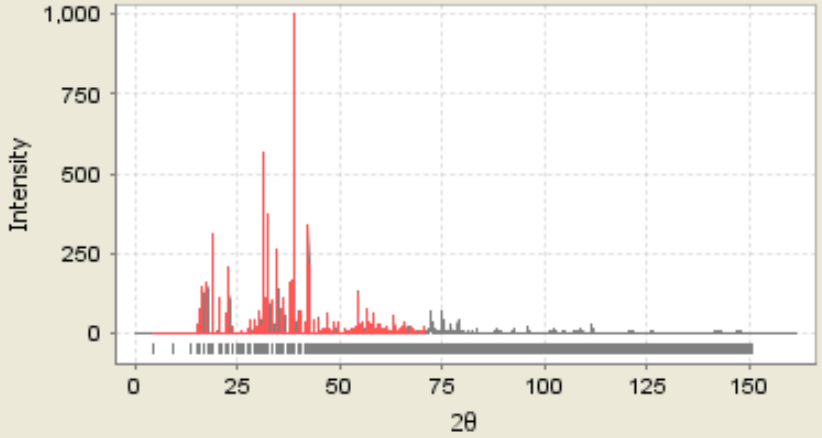
- [x] Fixed Slit Intensity
- [ ] Variable Slit Intensity
- [ ] Integrated Intensity

Diffraction Pattern

- [x] Calculated Pattern
- [ ] PD3 Pattern

Fixed Slit Intensity

2θ	d(Å)	I	h	k	l	*
4.5511	19.400000	1	2	0	0	
9.1093	9.700000	1	4	0	0	
13.6821	6.466670	1	6	0	0	
15.1921	5.827150	32	1	0	1	
15.7008	5.639470	75	2	0	1	
16.5147	5.363320	145	3	0	1	
17.5928	5.037030	163	4	0	1	
18.8913	4.693630	314	5	0	1	
20.3701	4.356100	113	6	0	1	
21.9950	4.037830	61	7	0	1	
22.9015	3.880000	206	10	0	0	



PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

PDF #: 04-007-1562 Status: Primary QM: Star (S)

Pressure/Temperature: Ambient

Chemical Formula: Ca Cu

Structural Formula:

Empirical Formula: Ca Cu

Weight %: Ca38.68 Cu61.32

Atomic %: Ca50.00 Cu50.00

ANX: NO

Compound Name: Calcium Copper

Mineral Name:

Common Name: α-Ca Cu

PDF Card - Ca Cu - 04-007-1562

File Edit d-Spacings Tools Window Help

d-Spacings

Wavelength

Cu Kα1 1.54056Å

Å

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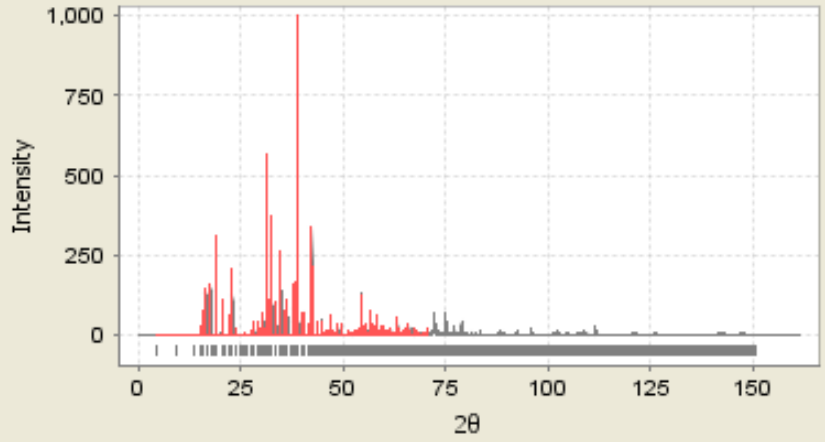
18.8913	4.693630	314	5	0	1	
20.3701	4.356100	113	6	0	1	
21.9950	4.037830	61	7	0	1	
22.9015	3.880000	206	10	0	0	



PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

Author's Reported Data (See Reference tab for source)

Radiation: CuKα1

λ: 1.5406 Å

Filter:

d-Spacing: Calculated

Cutoff:

Intensity: Calculated

I/Ic: 2.71

Camera Diameter:

PDF Card - Ca Cu - 04-007-1562

File Edit d-Spacings Tools Window Help

d-Spacings

Wavelength

Cu Kα1 1.54056Å

Å

Stick Pattern

- [x] Fixed Slit Intensity
- [ ] Variable Slit Intensity
- [ ] Integrated Intensity

Diffraction Pattern

- [x] Calculated Pattern
- [ ] PD3 Pattern

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15.1921	5.827150	32	1	0	1	
15.7008	5.639470	75	2	0	1	
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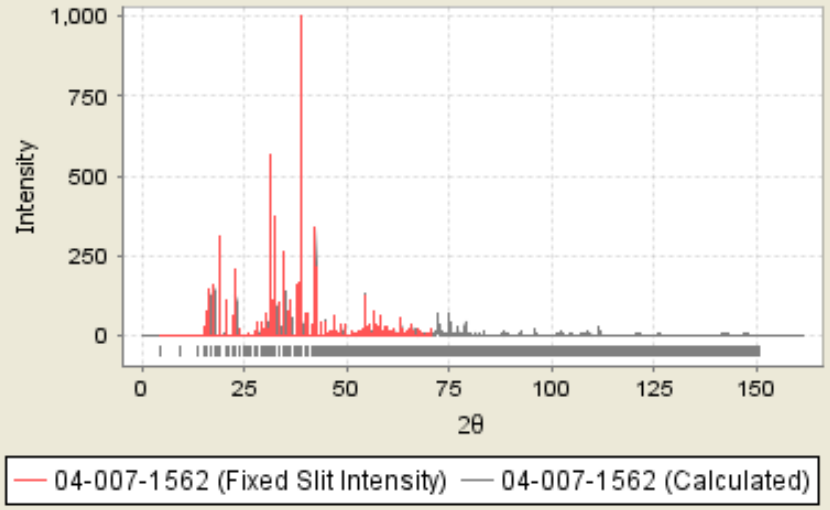
20.3701	4.356100	113	6	0	1	
21.9950	4.037830	61	7	0	1	
22.9015	3.880000	206	10	0	0	



PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

SYS: Orthorhombic Space Group: Pnma (62) Aspect:

Author's Cell (See Reference tab for source)

a: 38.80(1) Å b: 4.2710(20) Å c: 5.8940(90) Å

α: ° β: ° γ: °

Volume: 976.72 Å³ Z: 20.00 MolVol: 48.84

Convert Cell

Author's Cell Axial Ratio

c/a: 0.152 a/b: 9.085 c/b: 1.380

Dcalc: 3.524 g/cm³ Dmeas: g/cm³ Dstruc: 3.52 g/cm³

SS/FOM: F(30) = 148.2(0.0051, 40) Melting Point:

R-factor: 0.061 Error:

PDF Card - Ca Cu - 04-007-1562

File Edit d-Spacings Tools Window Help

d-Spacings

Wavelength

Cu Kα1 1.54056Å

Å

Stick Pattern

- [x] Fixed Slit Intensity
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- [ ] Integrated Intensity

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- [ ] PD3 Pattern

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15.1921	5.827150	32	1	0	1	
15.7008	5.639470	75	2	0	1	
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20.3701	4.356100	113	6	0	1	
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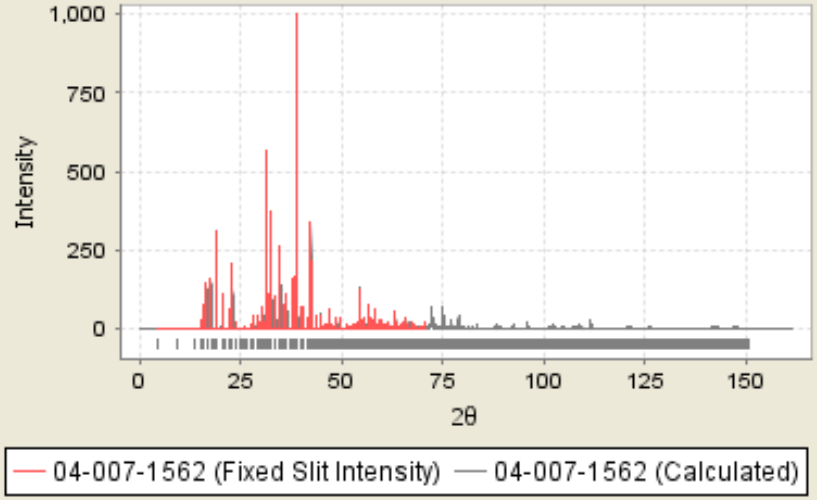
22.9015	3.880000	206	10	0	0	



PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

ICDD Calculated Parameters

Space Group: Pbnm (62)

Molecular Weight: 103.63

Crystal Data

a:	5.894 Å	b:	38.800 Å	c:	4.271 Å
α:	90.00 °	β:	90.00 °	γ:	90.00 °
Volume:	976.72 Å³	Z:	20.00		

Crystal Data Axial Ratio

c/a:	0.725	a/b:	0.152	c/b:	0.110

Reduced Cell

a:	4.271 Å	b:	5.894 Å	c:	38.800 Å
α:	90.00 °	β:	90.00 °	γ:	90.00 °
Volume:	976.72 Å³				

PDF Card - Ca Cu - 04-007-1562

File Edit d-Spacings Tools Window Help

d-Spacings

Wavelength

Cu Kα1 1.54056Å

Å

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- [ ] Integrated Intensity

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15.1921	5.827150	32	1	0	1	
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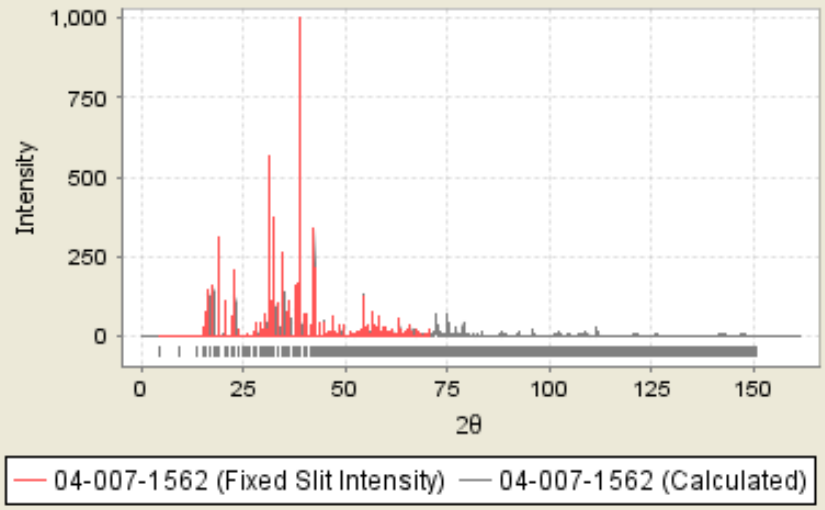
22.9015	3.880000	206	10	0	0	



PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

(See Reference tab for source)

εα: nωβ: εγ:

Sign: 2V:

PDF Card - Ca Cu - 04-007-1562

File Edit d-Spacings Tools Window Help

d-Spacings

Wavelength

Cu Kα1 1.54056Å

Å

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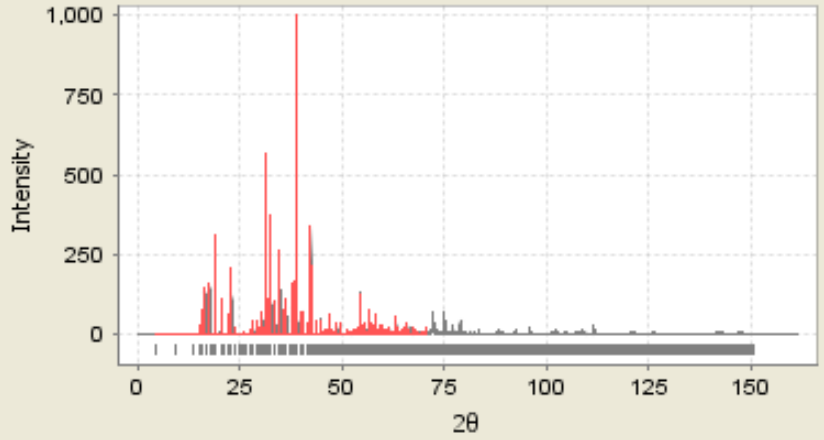
21.9950	4.037830	61	7	0	1	
22.9015	3.880000	206	10	0	0	



PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

SG Symmetry Operators (8)

Seq	Operator
1	x,y,z
2	-x,-y,-z
3	x+1/2,-y+1/2,-z+1/2
4	-x+1/2,y+1/2,z+1/2
5	-x,y+1/2,-z
6	x,-y+1/2,z
7	-x+1/2,-y,z+1/2
8	x+1/2,y,-z+1/2

TDP Type: U Origin: Crystal (Symmetry Allowed): Centrosymmetric

Atomic Coordinates (10)

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	IDP	AET
Ca	1	4c	.m.	0.4638	0.25	0.6321	1.0	0.02	17-d
Ca	2	4c	.m.	0.3652	0.25	0.8735	1.0	0.02	17-d
Ca	3	4c	.m.	0.2639	0.25	0.1259	1.0	0.02	17-d
Ca	4	4c	.m.	0.1644	0.25	0.8726	1.0	0.02	17-d

Anisotropic Thermal Displacement Parameters (0)

PDF Card - Ca Cu - 04-007-1562

File Edit d-Spacings Tools Window Help

d-Spacings

Wavelength

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Å

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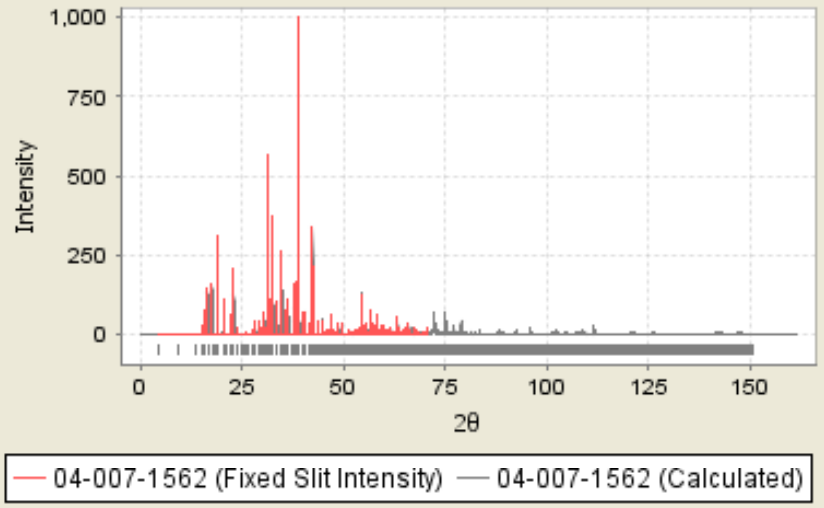
21.9950	4.037830	61	7	0	1	
22.9015	3.880000	206	10	0	0	



PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

CAS:

Pearson: oP40.00

Pearson w/o H:

Former PDF's #: 01-072-5678, 03-065-2256, 03-065-7630

Cross-Ref PDF #'s (1)

00-041-1273 (Primary)

Prototype Structure:

Prototype Structure (Alpha Order):

LPF Prototype Structure: Ca Cu,oP40,62

LPF Prototype Structure (Alpha Order): Ca Cu

Mineral Classification:

Zeolite Classification:

Subfile(s): LPF Pattern, Metals & Alloys, Primary Pattern, Inorganic

Entry Date: 01/05/2005

Last Modification Date: 01/25/2010

PDF Card - Ca Cu - 04-007-1562

File Edit d-Spacings Tools Window Help

d-Spacings

Wavelength

Cu Kα1 1.54056Å

Å

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- [ ] Integrated Intensity

Diffraction Pattern

- [x] Calculated Pattern
- [ ] PD3 Pattern

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15.7008	5.639470	75	2	0	1	
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21.9950	4.037830	61	7	0	1	
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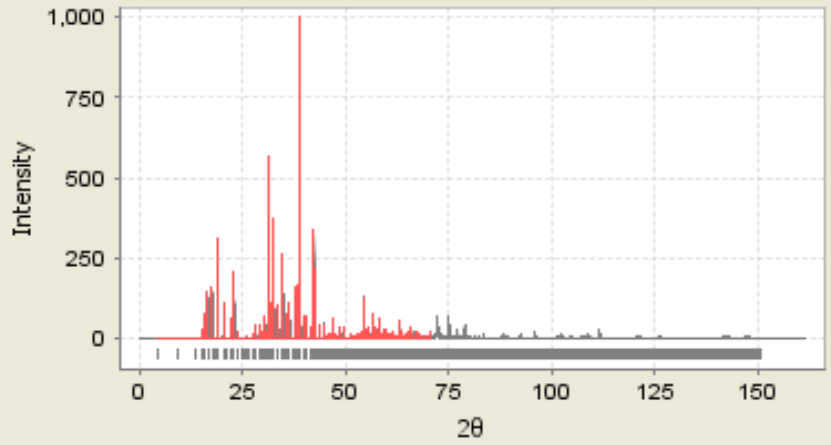

PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

Experimental Data Reference

"The Structures of α-CaCu, β-CaCu, SrAg and BaAg: Four Different Stacking Variants Based on Noble-Metal-Centred Trigonal Prisms". Merlo F., Fornasini M.L. *Acta Crystallogr., Sec. B: Struct. Crystallogr. Cryst. Chem.* **37**, 500 (1981). Calculated from LPF using POWD-12++.

Additional Powder Data Reference(s)

Physical Data Reference(s)

Ibid.

Optical Data Reference(s)

PDF Card - Ca Cu - 04-007-1562

File Edit d-Spacings Tools Window Help

d-Spacings

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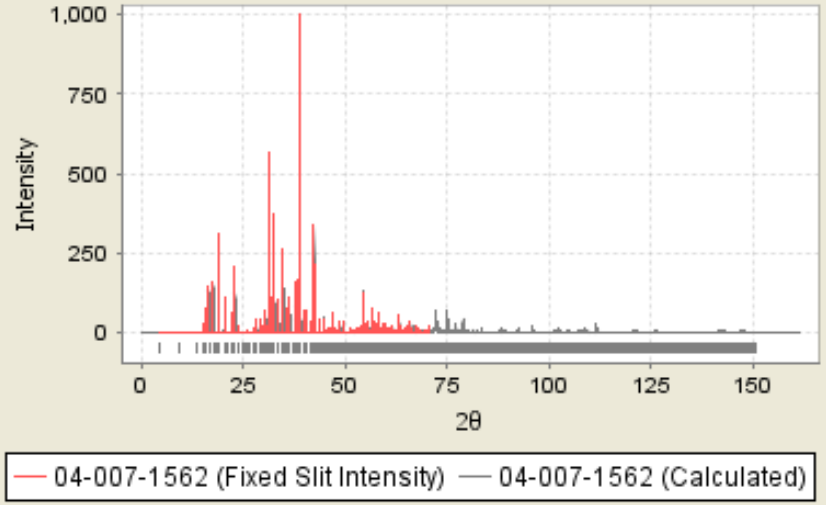
21.9950	4.037830	61	7	0	1	
22.9015	3.880000	206	10	0	0	



PDF | Experimental | Physical | Crystal | Optical | Structure | Miscellaneous | References | Comments

Database Comments

ANX: NO. LPF Collection Code: 1251296. Sample Preparation: STARTING MATERIALS:Ca,Cu. Compound Preparation: melted, water-quenched from 873 K. CRUCIBLE: iron. ATMOSPHERE: argon. Unit Cell Data Source: Single Crystal.

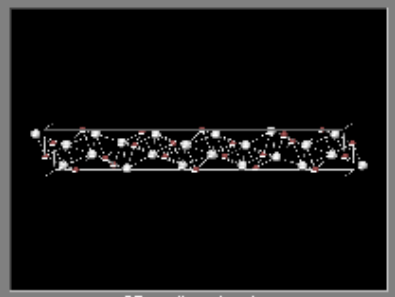
User Comments

Save Comment

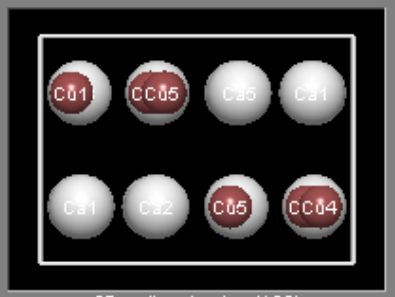
Shared Comments

040071562 :Ca Cu - 3D

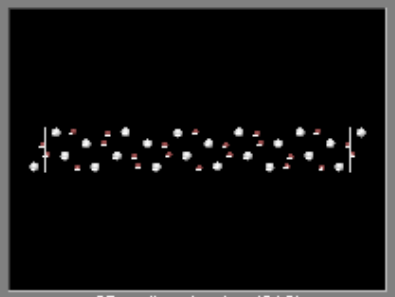
File Option



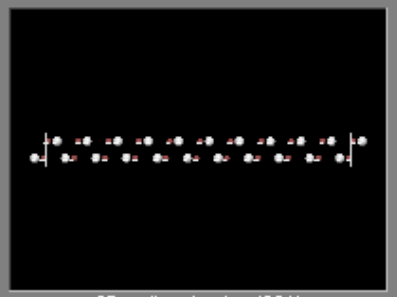
3D cell projection



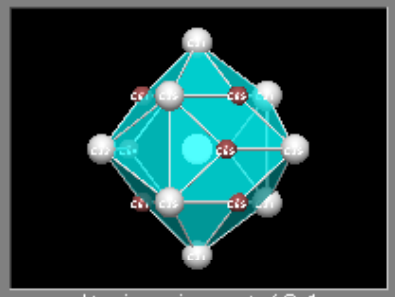
2D cell projection (100)



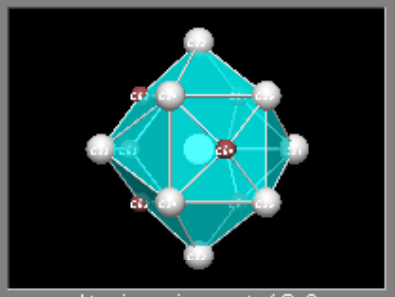
2D cell projection (010)



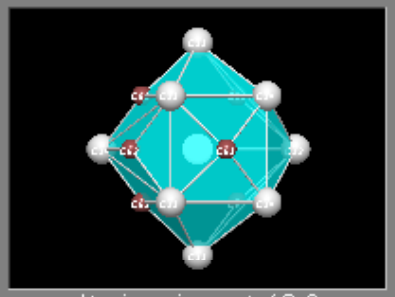
2D cell projection (001)



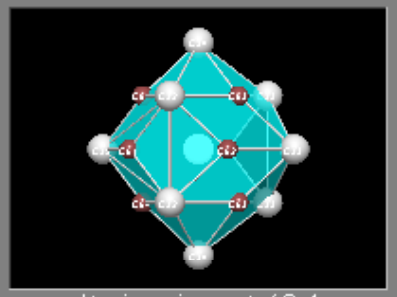
Atomic environment of Ca1



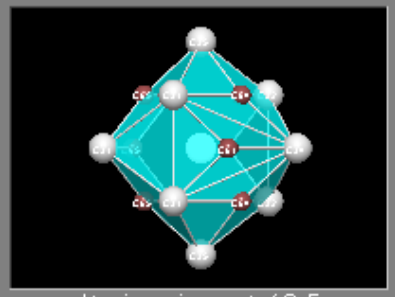
Atomic environment of Ca2



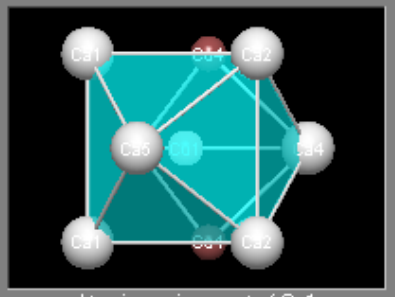
Atomic environment of Ca3



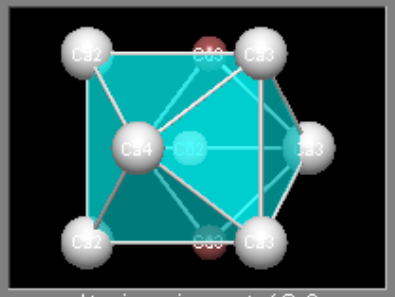
Atomic environment of Ca4



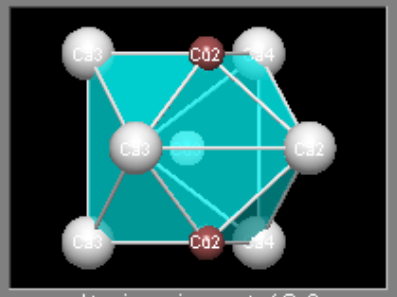
Atomic environment of Ca5



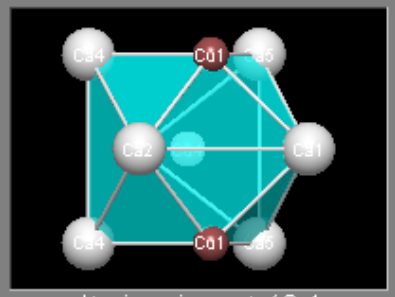
Atomic environment of Cu1



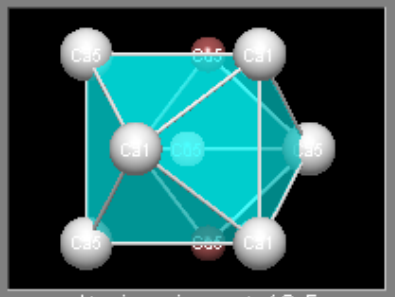
Atomic environment of Cu2



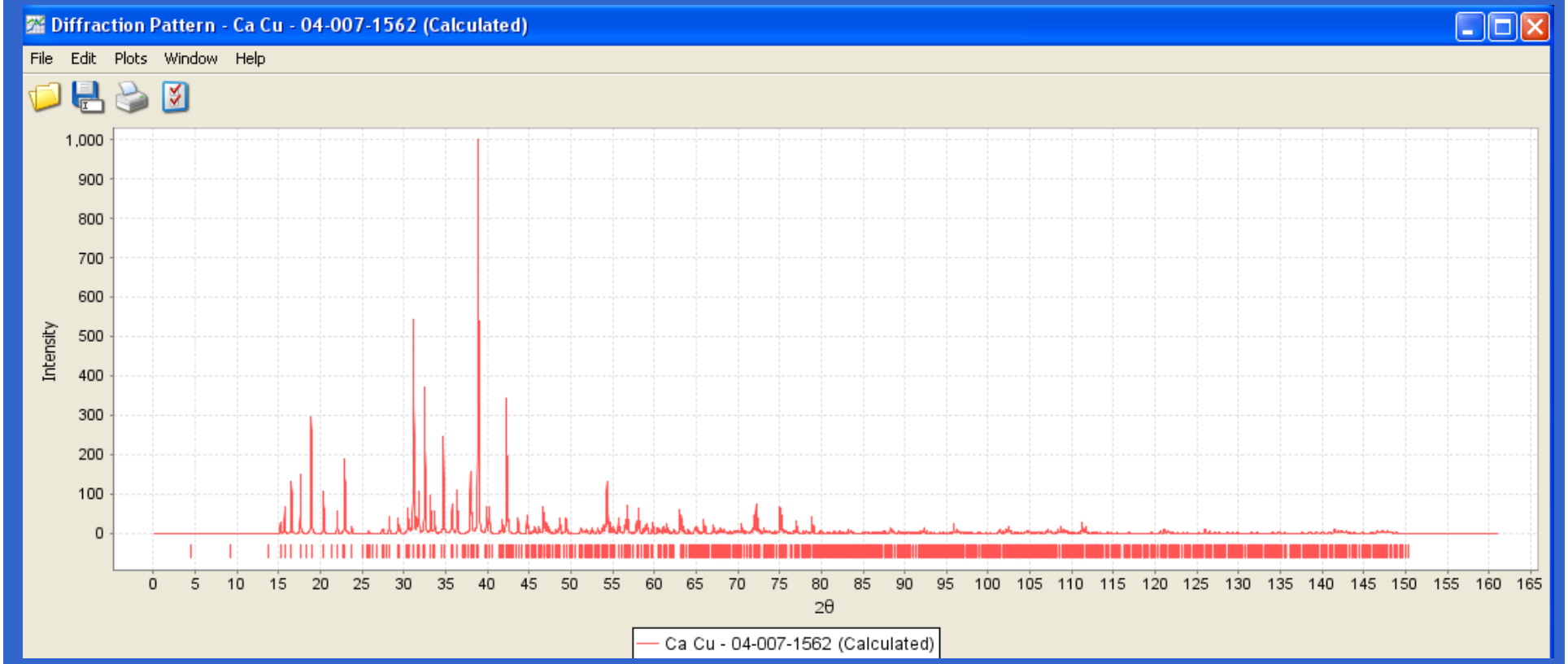
Atomic environment of Cu3



Atomic environment of Cu4

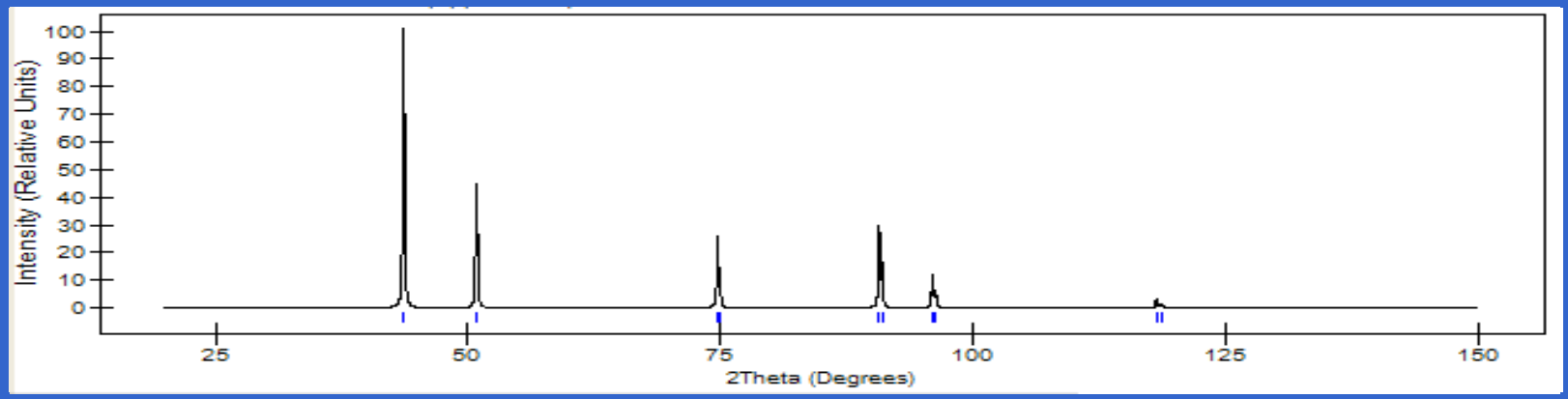


Atomic environment of Cu5


Diffraction Pattern - Ca Cu - 04-007-1562 (Calculated)
File
Edit
Plots
Window
Help
Intensity
1,000
900
800
700
600
500
400
300
200
100
0
0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165
2θ
Ca Cu - 04-007-1562 (Calculated)

Powder diffraction - applications

Qualitative analysis - what IS this stuff?!!



Make d, I list:

Do search/match

2.080	100	1	1.081	30	6
2.025	100	2	1.040	12	
1.798	45	4	1.018	20	8
1.433	20		0.907	35	5
1.272	26	7	0.898	3	
1.170	50	3	0.830	14	

Powder diffraction - applications

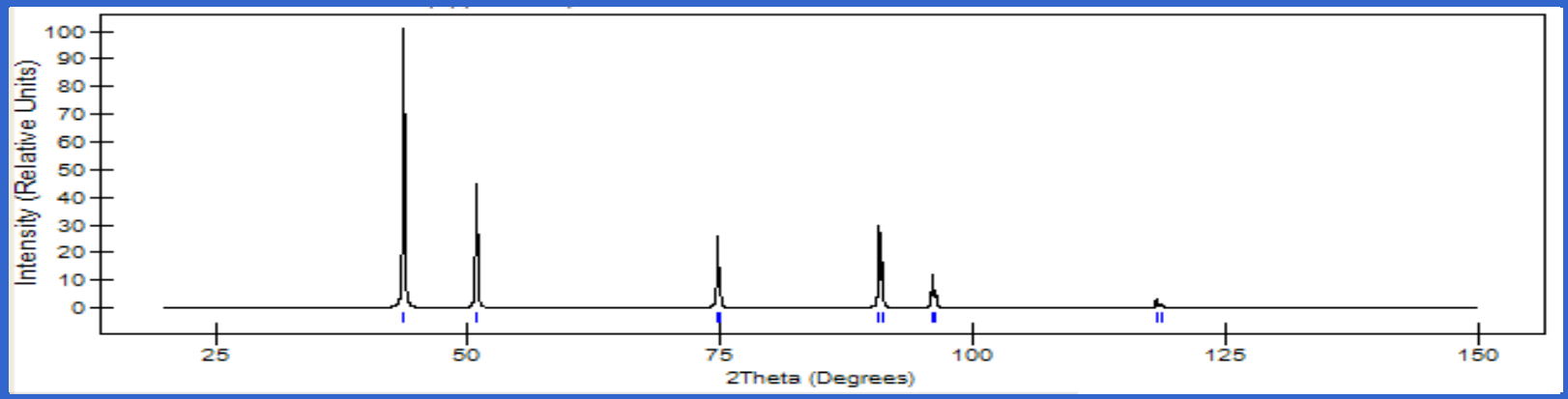
Qualitative analysis - what IS this stuff?!!

Example of page of search manual for Hanawalt manual search/match

3.39 – 3.32 (±.02)									File No.
3.38_9	8.58_X	3.04_9	4.11_8	3.18_8	1.69_7	2.65_6	1.88_5	$(Mg,Fe)_2Al_4Si_5O_{18}$/Cordierite, ferroan	9– 472
3.33_X	6.72_9	3.19_8	8.09_7	3.28_7	5.18_4	3.10_4	4.30_4	$C_{10}H_{10}N_2O_6$	29–1716
3.31_8	6.40_X	6.10_8	3.85_5	2.77_5	6.70_4	3.48_4	2.64_4	$C_{12}H_6Cl_6$	17–1054
3.38_9	6.13_X	8.66_9	3.20_9	3.29_5	9.70_3	4.57_3	3.46_3	$C_{11}H_{11}N_3 \cdot HCl$	28–1749
3.34_X	5.93_2	5.19_1	3.77_1	3.65_1	3.51_1	2.94_1	1.67_1	$C_4H_8N_2O_2$	26–1863
3.37_X	5.85_9	3.86_9	3.72_7	3.52_7	3.03_7	2.70_7	7.72_6	$C_4H_9N_2O_2 \cdot HCl$	5– 459
3.31_8	5.73_X	3.43_7	3.59_6	3.19_5	4.36_4	4.19_3	3.27_3	$C_6H_5NO_2$	30–1845
3.30_X	5.44_7	5.63_5	3.24_4	4.97_3	6.58_3	4.58_2	3.15_2	$(NH_4)_4P_2O_7$	20– 102
3.38_X	5.30_X	3.49_X	5.90_3	3.67_3	3.26_3	3.18_3	2.99_3	$KH_3P_2O_7$	15– 509
3.35_X	5.21_8	4.86_8	4.33_8	4.04_8	3.90_8	3.55_8	2.73_8	β-$C_9H_{11}NO_2$	22–1874
3.40_X	5.01_9	3.09_7	4.10_4	3.00_4	4.03_3	6.74_2	3.45_2	$C_3H_4N_6$	24–1654
3.30_X	4.76_6	4.18_6	5.73_3	2.92_3	3.98_3	2.38_2	3.35_2	$C_8H_6O_4$	37–1919
3.31_X	4.71_8	3.50_8	5.56_3	3.84_3	3.03_3	7.02_2	2.30_2	$C_6H_5NO_2 \cdot HCl$	29–1827
3.39_X	4.48_5	3.43_5	3.01_5	4.09_4	2.98_4	2.78_4	3.18_3	$NaHSO_4$	25– 833
3.34_9	4.42_X	10.1_9	1.48_9	2.56_8	1.68_8	1.28_7	1.23_7	$Al_2Si_2O_5(OH)_4 \cdot 2H_2O$/Halloysite-10A	9– 451
3.40_9	4.38_X	2.88_7	5.76_4	2.61_4	4.09_4	2.76_4	1.76_3	V_2O_5/Shcherbinaite, syn	9– 387
3.33_X	4.30_5	2.82_5	6.08_2	4.72_2	1.71_1	3.52_1	2.15_1	$(NH_4)_2Ca_2(SO_4)_3$	22–1037
3.37_X	4.28_3	1.84_2	1.55_1	2.47_1	2.31_1	1.39_1	2.14_1	$AlPO_4$/Berlinite, syn	10– 423
3.34_X	4.26_3	1.82_1	1.54_1	2.46_1	2.28_1	1.37_1	1.38_1	SiO_2/Quartz, low, syn	33–1161
3.36_X	4.23_X	3.57_7	5.27_4	3.72_4	4.04_4	3.97_3	7.19_2	$C_6H_8N_2O_2S$	30–1944

Powder diffraction - applications

Qualitative analysis - what IS this stuff?!!



Make d, I list:

2.080	100	1	1.081	30	6
2.025	100	2	1.040	12	
1.798	45	4	1.018	20	8
1.433	20		0.907	35	5
1.272	26	7	0.898	3	
1.170	50	3	0.830	14	

Do search/match

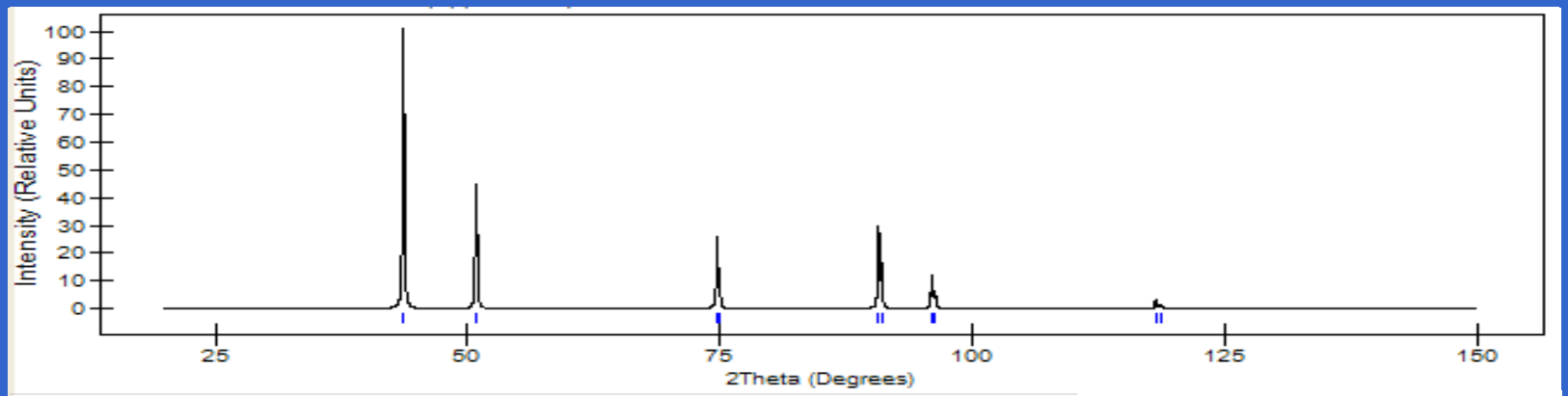
1 2 5 - no match

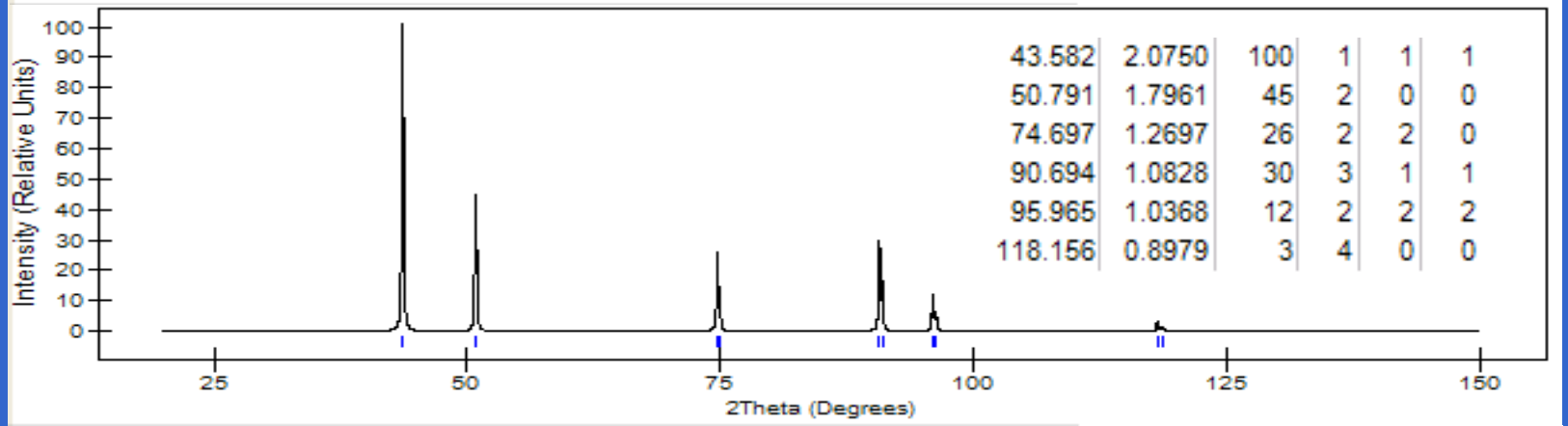
1 2 5 - MATCH!

1 3 x - no match

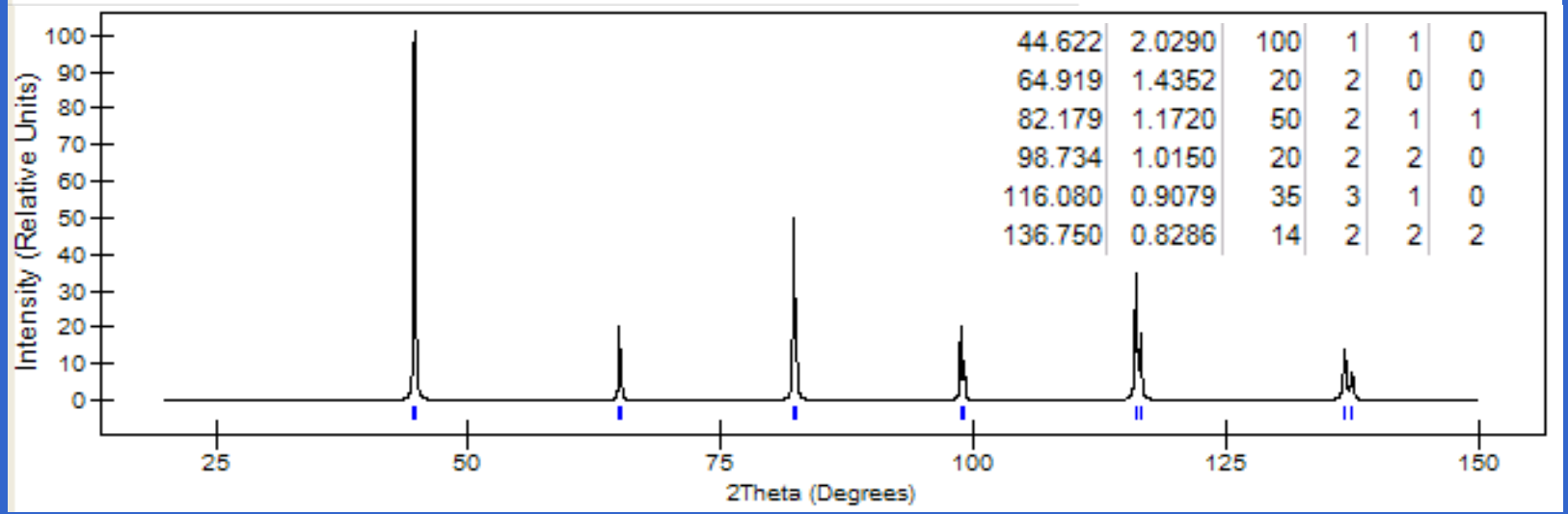
2.0750	100
1.7961	45
1.2697	26
1.0828	30
1.0368	12
0.8979	3

2.0290	100
1.4352	20
1.1720	50
1.0150	20
0.9079	35
0.8286	14





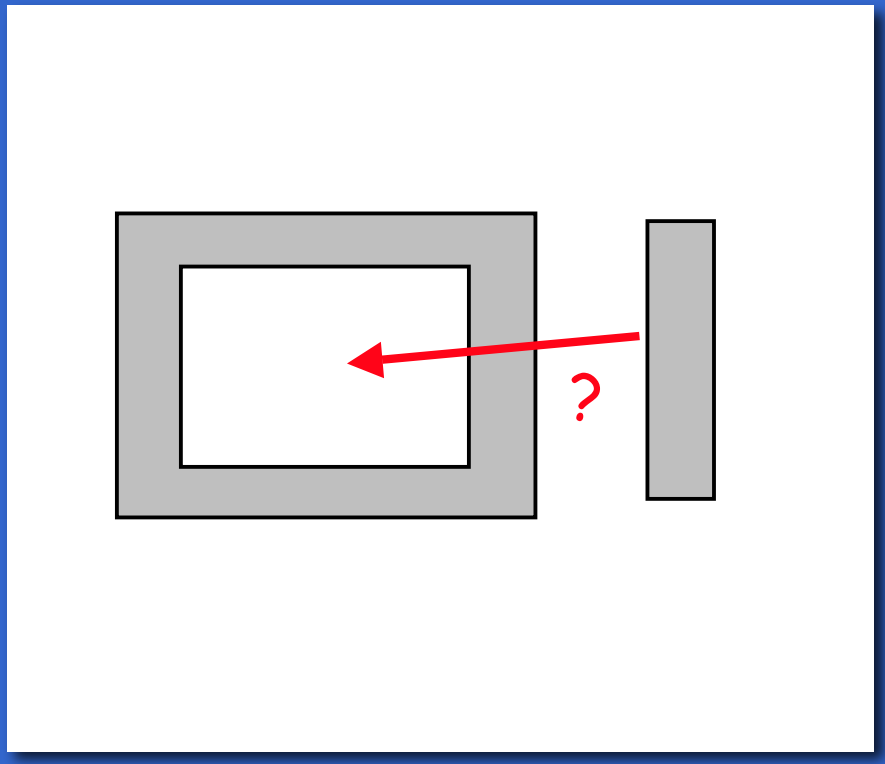
43.582	2.0750	100	1	1	1
50.791	1.7961	45	2	0	0
74.697	1.2697	26	2	2	0
90.694	1.0828	30	3	1	1
95.965	1.0368	12	2	2	2
118.156	0.8979	3	4	0	0



44.622	2.0290	100	1	1	0
64.919	1.4352	20	2	0	0
82.179	1.1720	50	2	1	1
98.734	1.0150	20	2	2	0
116.080	0.9079	35	3	1	0
136.750	0.8286	14	2	2	2

Powder diffraction - applications

1. Qualitative analysis
2. Quantitative analysis
3. Crystal structure determination
4. Crystallite size
5. Microstrain
6. Residual macrostresses 残余宏观应力



Powder diffraction - applications

1. Qualitative analysis
2. Quantitative analysis
3. Crystal structure determination
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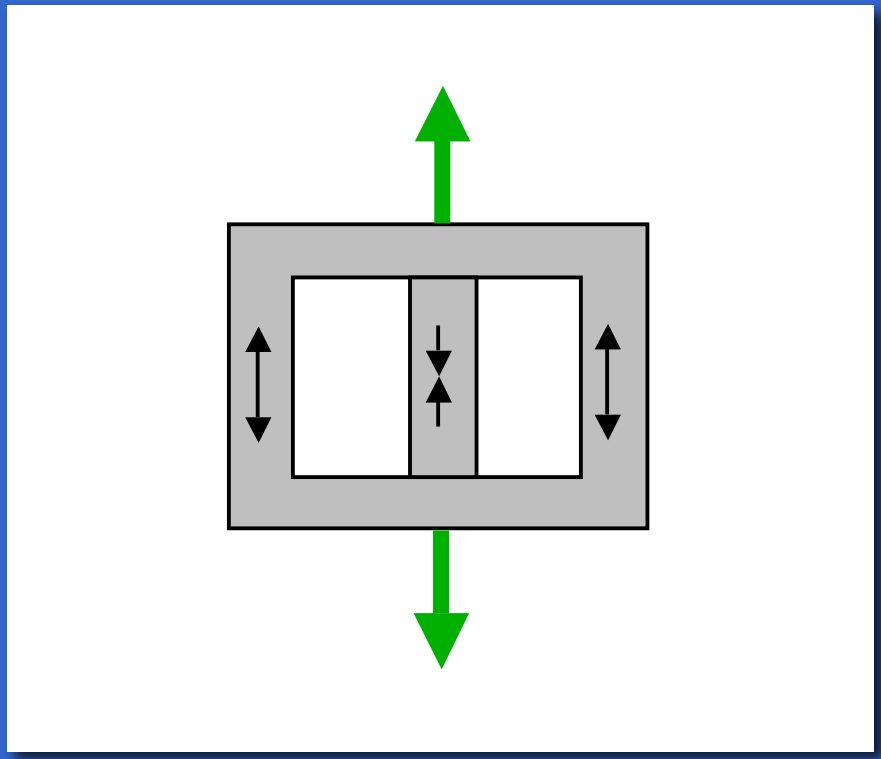
6. Residual macrostresses



stress = modulus x strain

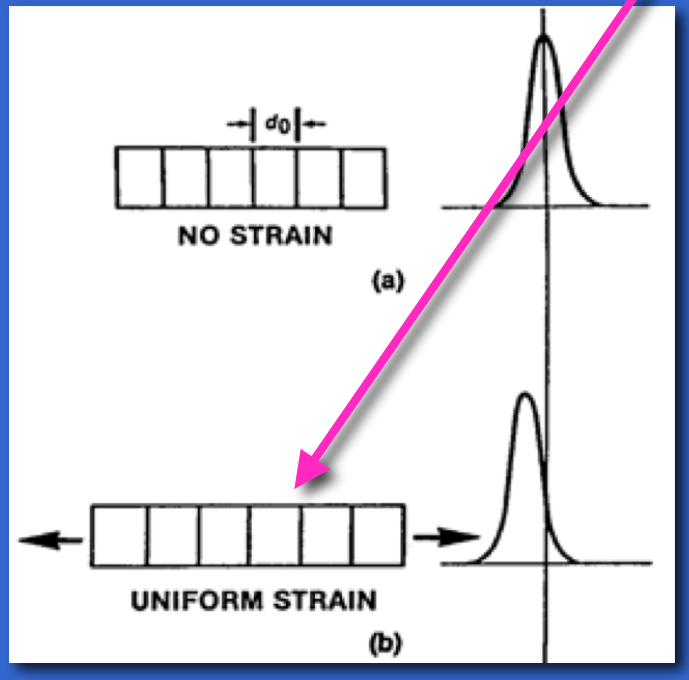
$\sigma = E\,\varepsilon$

(Hooke's law)

Powder diffraction - applications

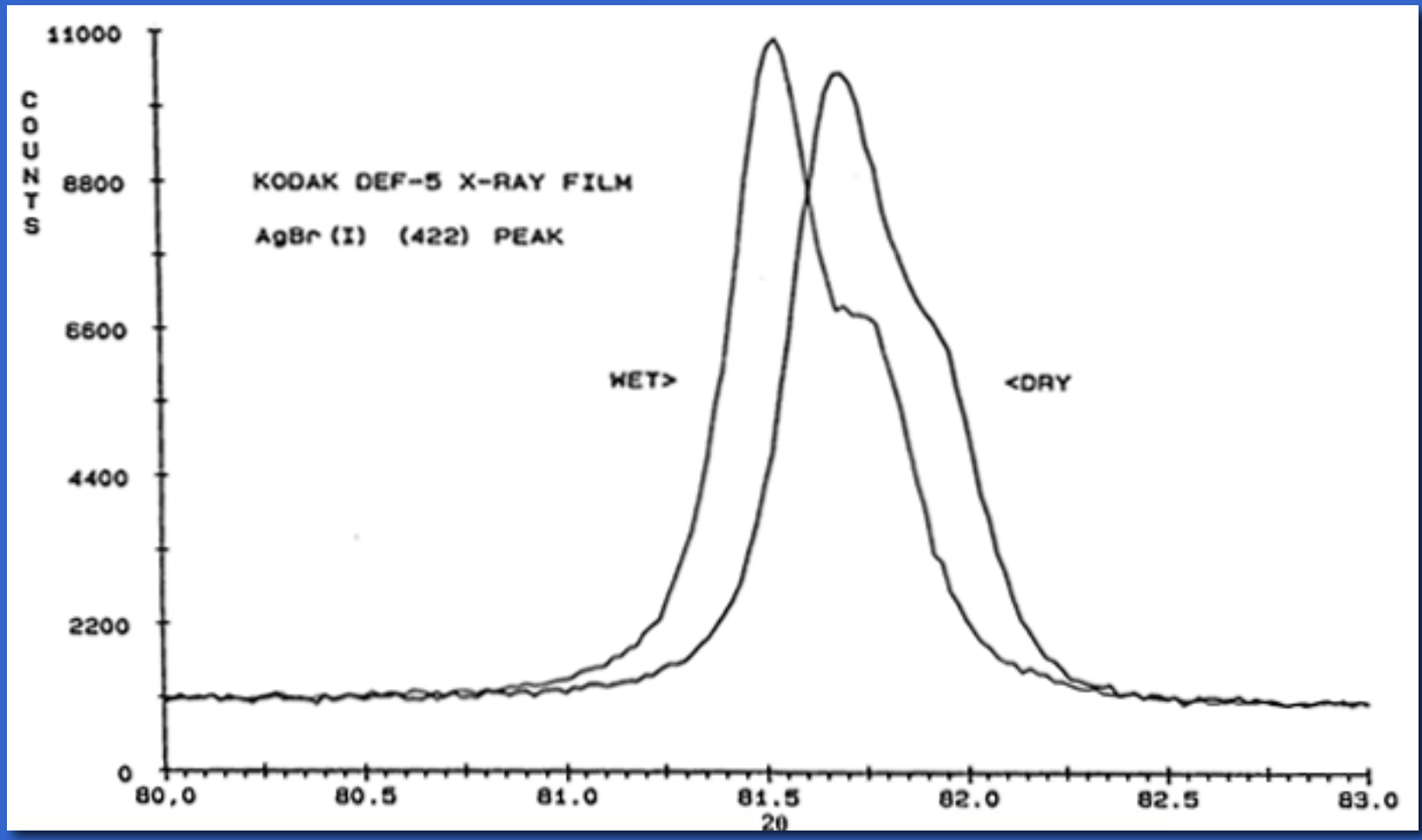
Residual stress

Reflections shift position (d-values change under stress)



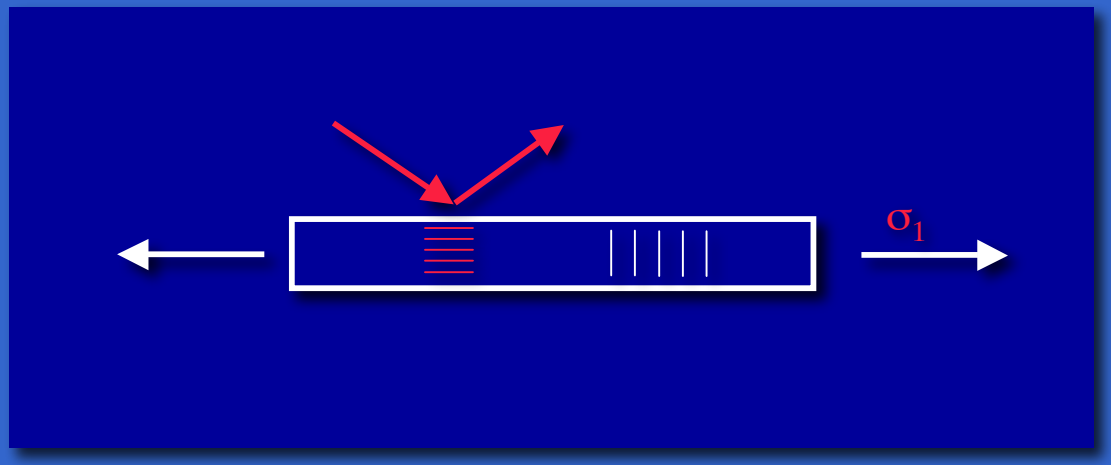
Powder diffraction - applications

Residual stresses



Residual stress

Suppose isotropic各向同性的 solid loaded in uniaxial 单轴的 tension



Can measure change in interplanar spacing for planes reflecting as above

$\Delta d = (d - d_o)/ d_o$ - this is the strain ε_3

$\varepsilon_3 = (1/E) (\sigma_3 - \nu(\sigma_1 + \sigma_2))$ - ν is Poisson's ratio

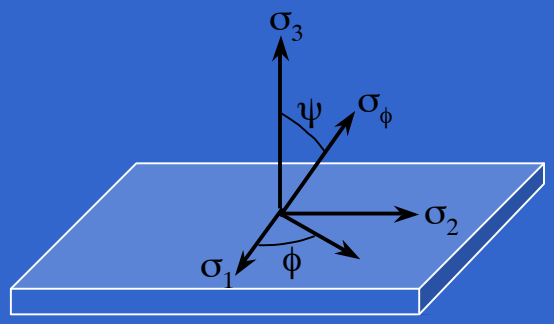
$\varepsilon_3 = - (1/E) \nu \sigma_1$ - so, can get stress

Residual stress

Biaxial & triaxial stress states more complicated
二軸　　三軸

Stress state resolved differently along different directions in sample, so peak shifts change w/ direction

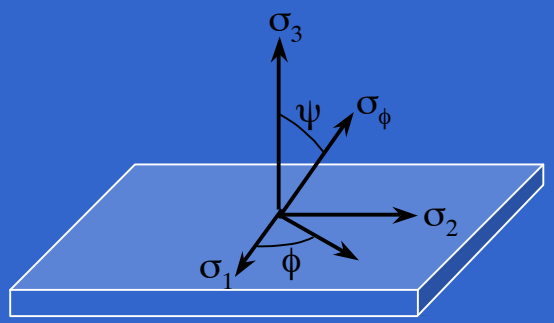
$$\varepsilon_{\phi\psi} = \sigma_{\phi}\,(1 + \nu)/E \sin^2\psi - (\nu/E)(\sigma_1 + \sigma_2)$$

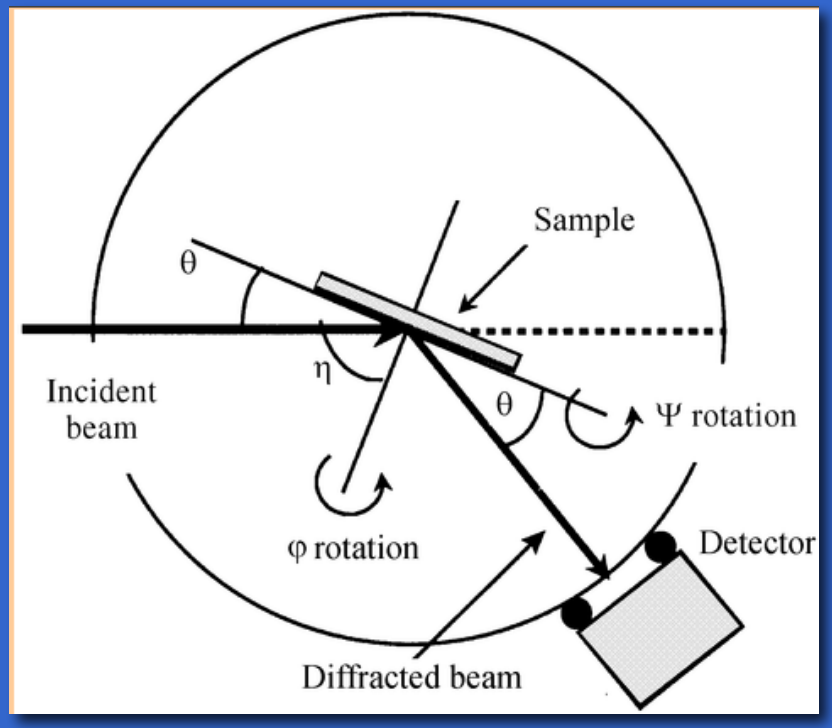


Residual stress

Measurement procedure - classical technique - $\sin^2 \psi$

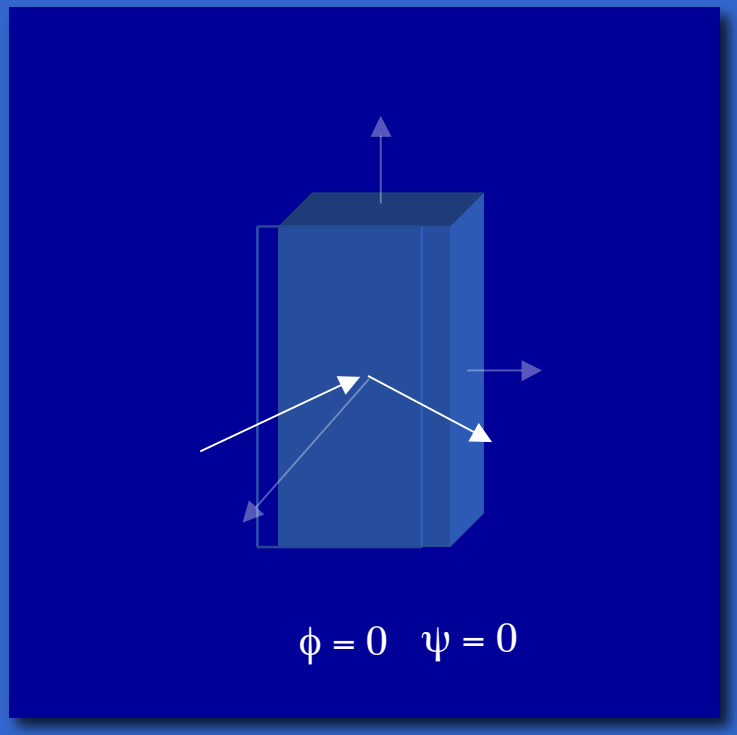
Diffractometer must have two more rotations - ϕ and ψ



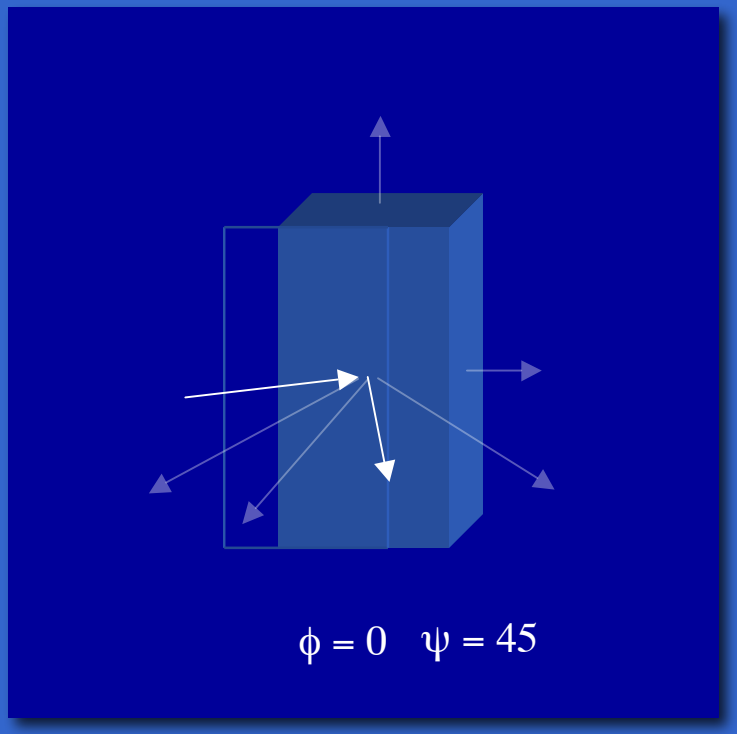


Residual stress

Measurement procedure - classical technique - $\sin^2 \psi$



$\phi = 0 \quad \psi = 0$

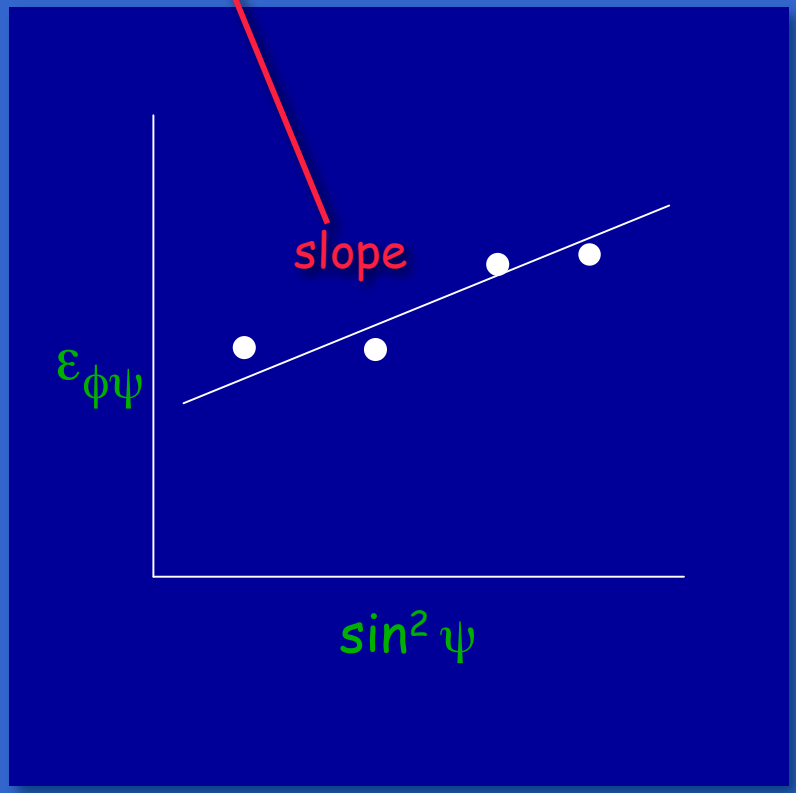


$\phi = 0 \quad \psi = 45$

Residual stress

Measurement procedure - classical technique - $\sin^2 \psi$

$$\varepsilon_{\phi\psi} = \sigma_\phi (1 + \nu)/E \sin^2 \psi - (\nu/E)(\sigma_1 + \sigma_2)$$



Need E, ν - measure or calculate

Powder diffraction - applications

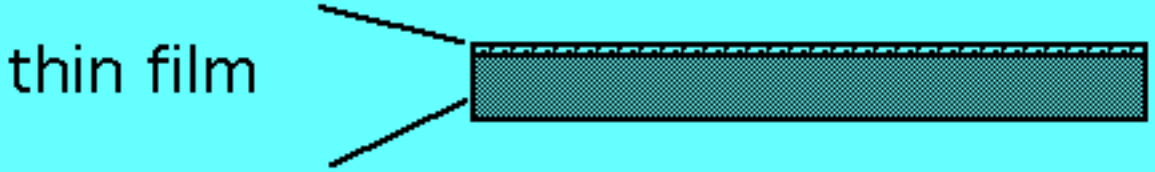
1. Qualitative analysis
2. Quantitative analysis
3. Crystal structure determination
4. Crystallite size
5. Microstrain
6. Residual macrostresses
7. Thin films

Powder diffraction - applications

Thin films

Epitaxy in polycrystalline thin films

外延



substrate

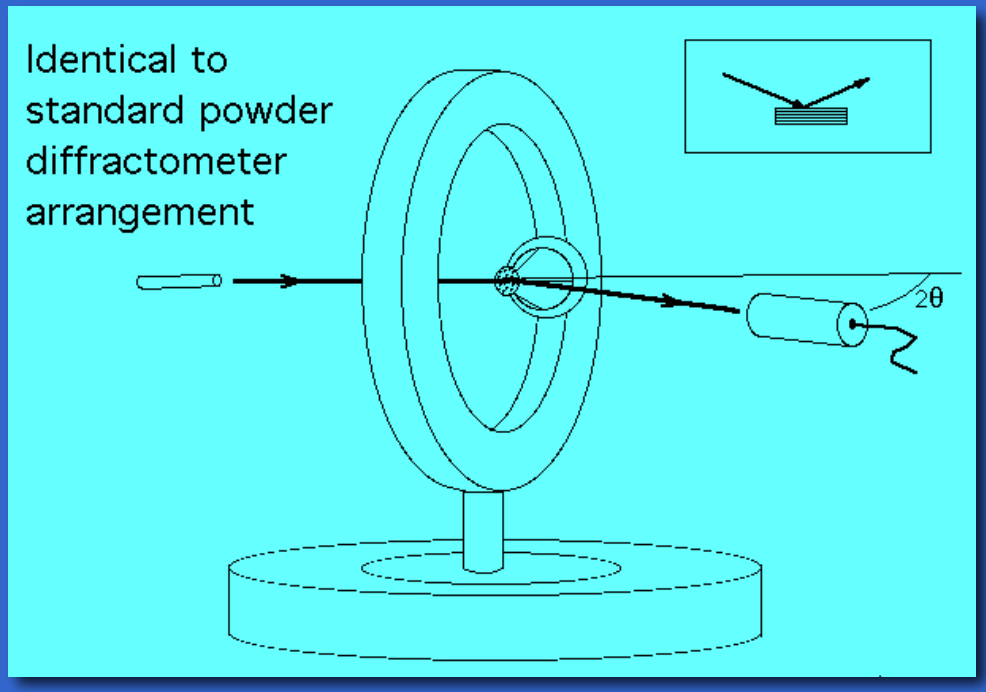
Powder diffraction - applications

Thin films

First, suppose we have a thin single crystal plate

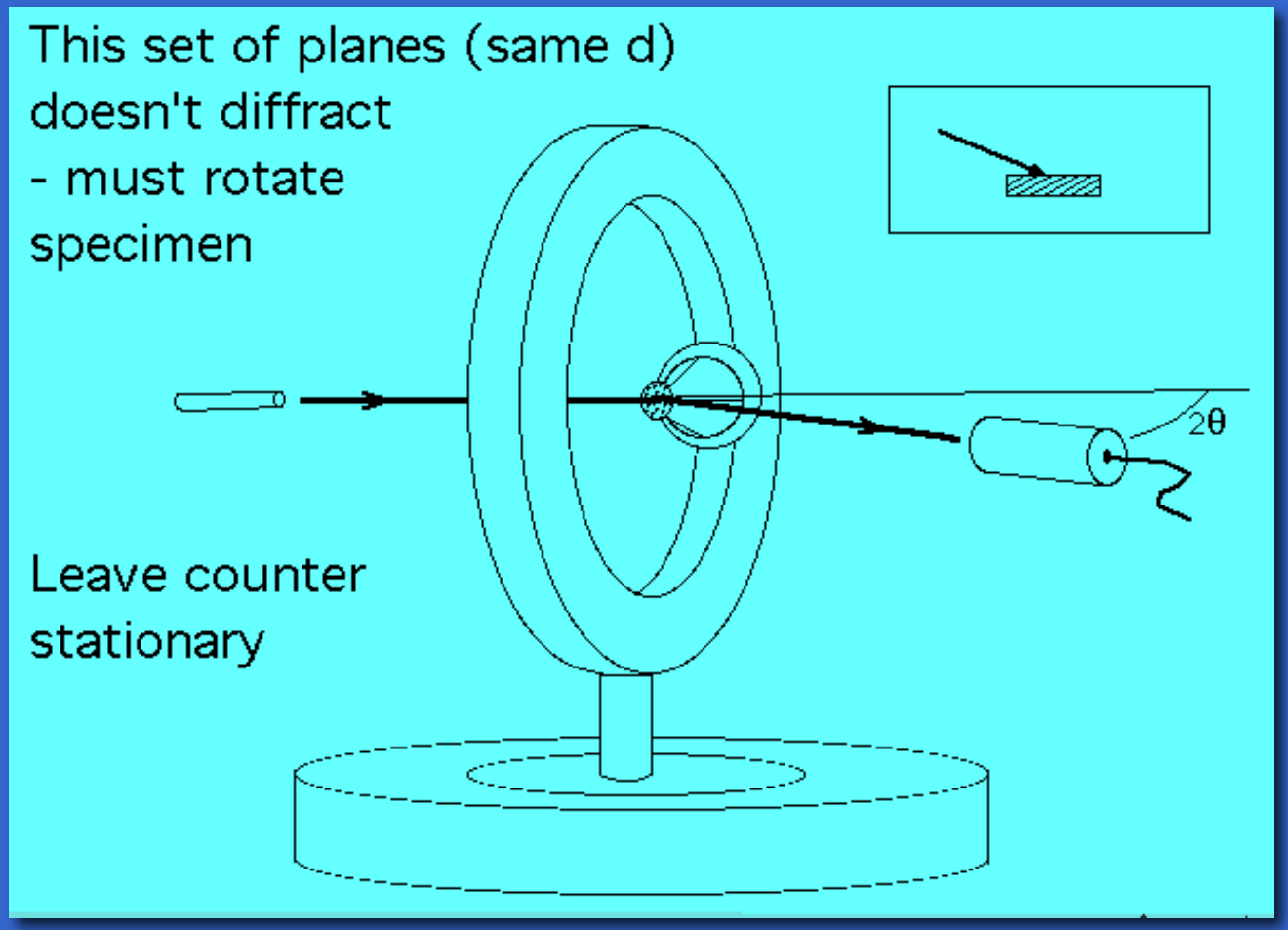
Mount in 4-circle diffractometer

Identical to standard powder diffractometer arrangement



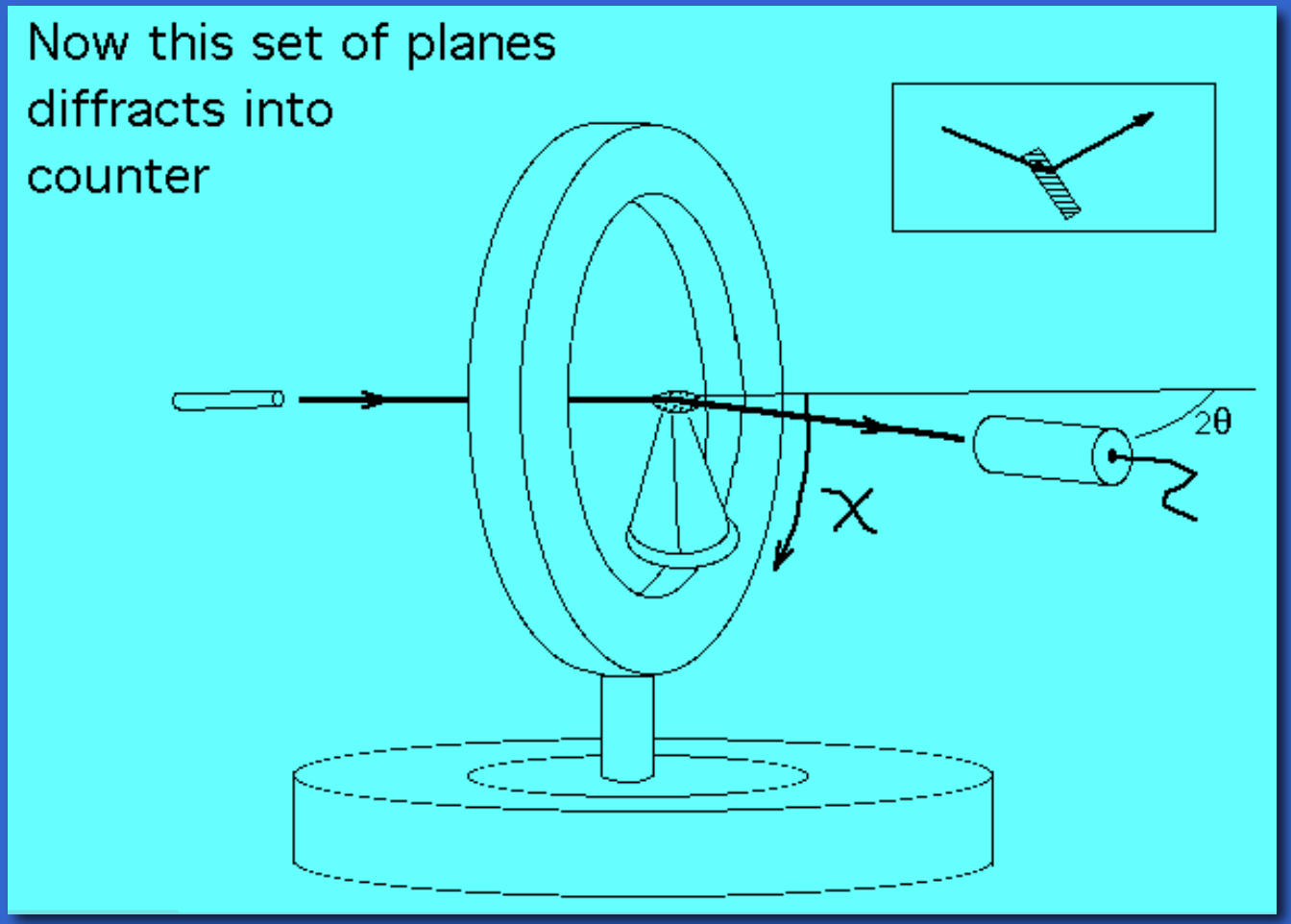
Powder diffraction - applications

Thin films



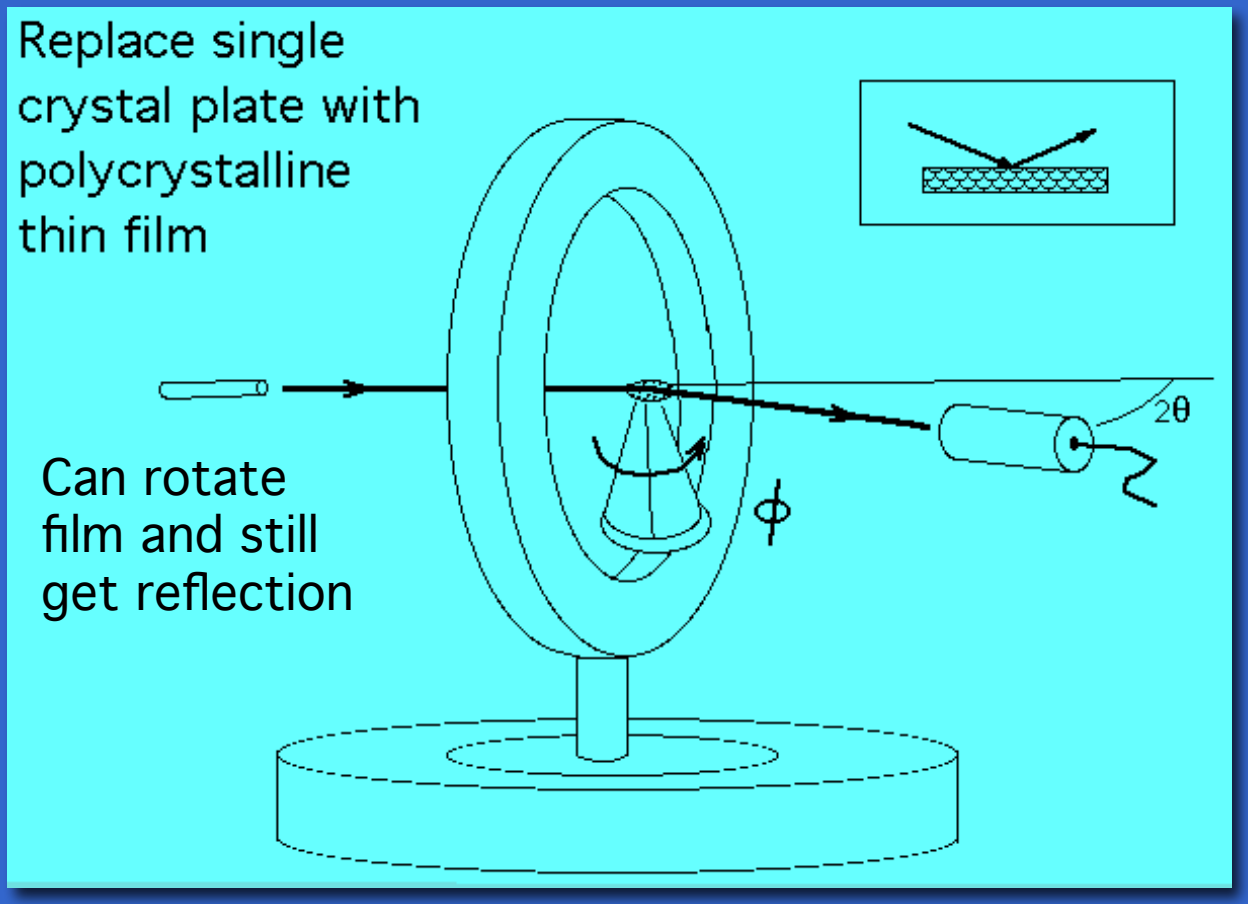
Powder diffraction - applications

Thin films



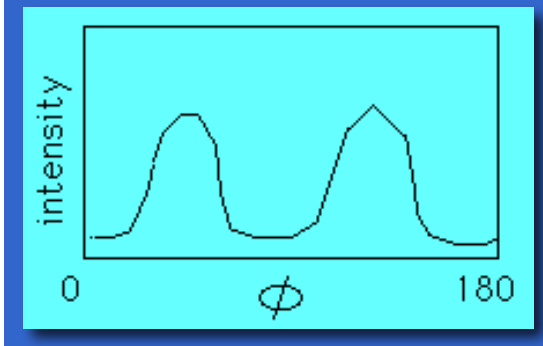
Powder diffraction - applications

Thin films

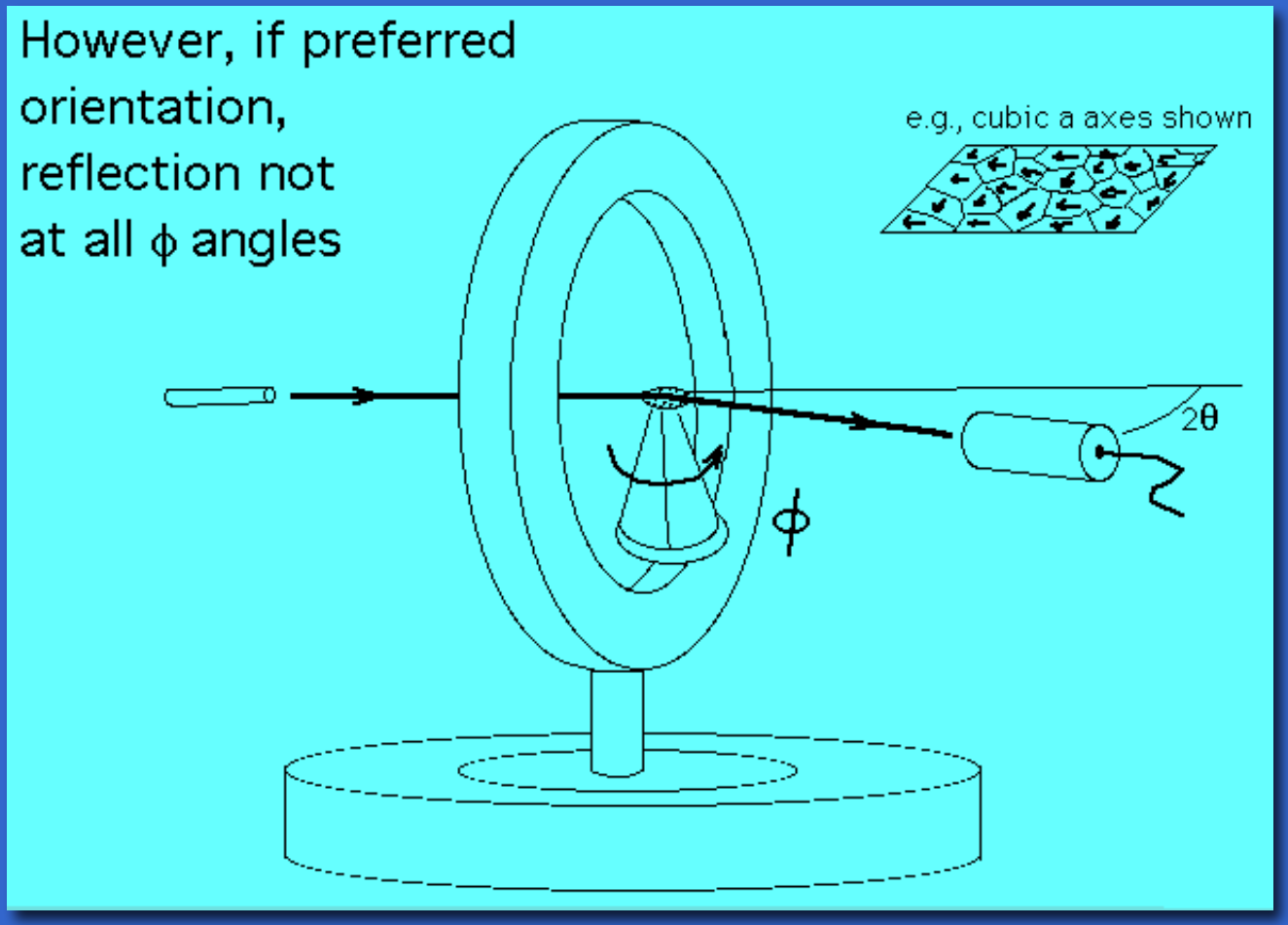


Powder diffraction - applications

Thin films



However, if preferred orientation, reflection not at all ϕ angles



Powder diffraction - applications

1. Qualitative analysis
2. Quantitative analysis
3. Crystal structure determination
4. Crystallite size
5. Microstrain
6. Residual macrostresses
7. Thin films
8. Crystallinity
9. Studies of phase diagrams
    A. Phase boundaries
    B. Solid solutions
    C. Phase transitions
10. Studies of chemical reactions and identification of reaction products.
11. Determination of grain sizes.
12. Preferred orientation in polycrystalline bodies.
13. Many more