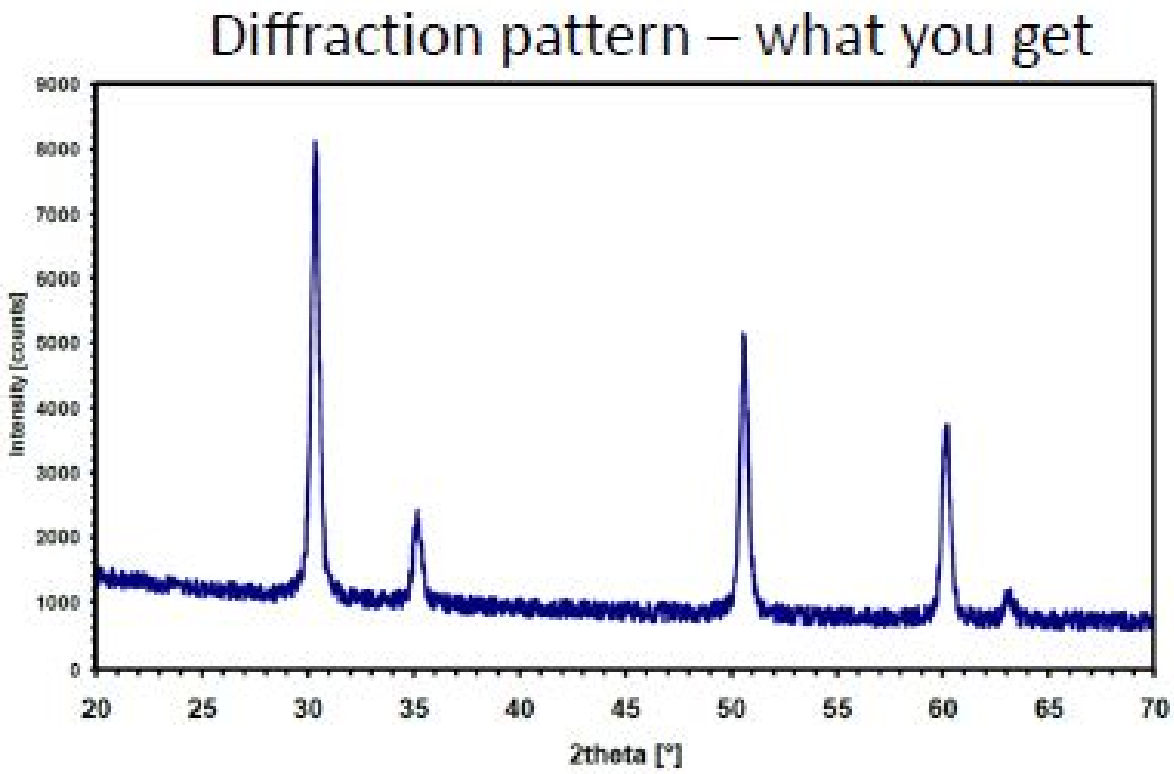
Lattice parameter 결정



Cubic system

Peak position, 2θ → d-spacing → unit cell parameter, a

$\lambda = 2d_{hkl} \sin \theta_{hkl}$

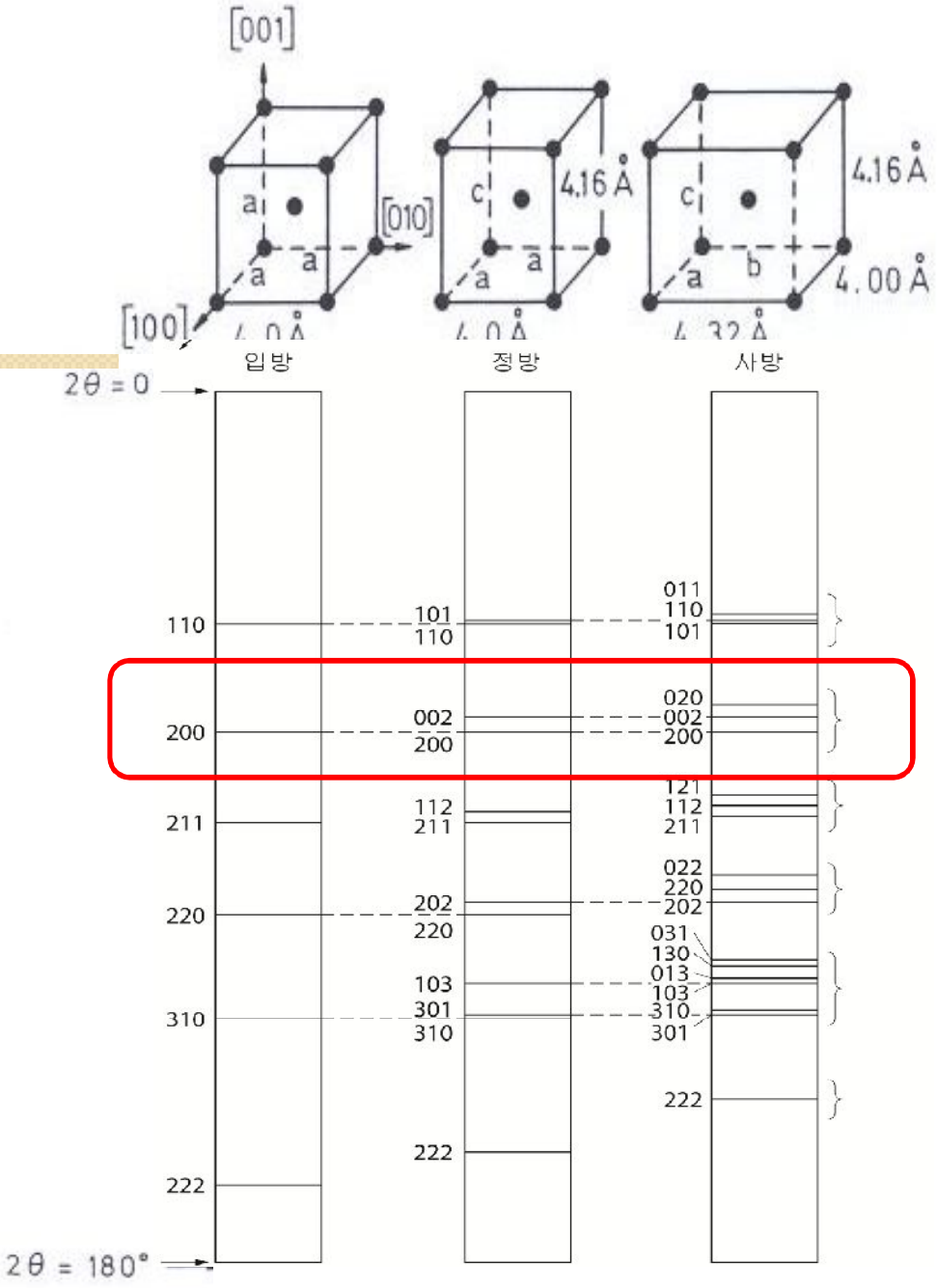
$1/d = 2 \sin\theta / \lambda$

$1/d^2 = 4 \sin^2\theta / \lambda^2$

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

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

10-5 분말무늬에 미치는 단위포 변형의 영향



Cubic, a=b=c

→[001]축 4% 증가
tetragonal, a=b≠c

→[010] 축 8% 증가
orthorhombic, a≠b≠c

d_{002}
d_{200}
d_{020}

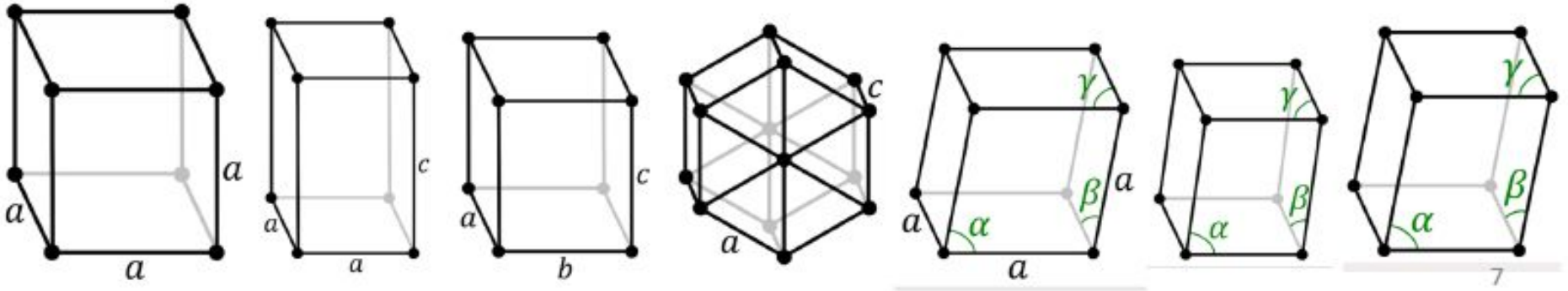
Cubic, $d_{002}=d_{200}=d_{020}$

Tetragonal, $d_{002} \neq d_{200}=d_{020}$

Orthorhombic, $d_{002} \neq d_{200} \neq d_{020}$

Crystal system	Cell lengths	Cell angles
Cubic	a=b=c	α=β=γ=90°
Tetragonal	a=b, c	α=β=γ=90°
Orthorhombic	a, b, c	α=β=γ=90°
Hexagonal	a=b, c	α=β=90°, γ=120°
Rhombohedral	a=b=c	α=β=γ
Monoclinic	a, b, c	α, β=γ=90°
Triclinic	a, b, c	α, β, γ

Decreasing symmetry



Decrease symmetry → (cubic --- triclinic) → reflection 증가

3-3 문제 풀이

(a) (100), (110), (111)

(b) (001), (100), (101)

(c) (100),(110), (001)

3-3 문제 풀이

(a) (100) 29.78, (110) 42.62, (111) 52.86

(b) (001) 29.78, (100) 45.34, (101) 61.86

(c) (100) 29.78,(110) 42.62, (001) 45.34