How to find Bravais lattice from x-ray scattering data.

(0. know your x-ray wavelength)

1. measure scattering angles 2θ

2. calculate lattice plane spacing

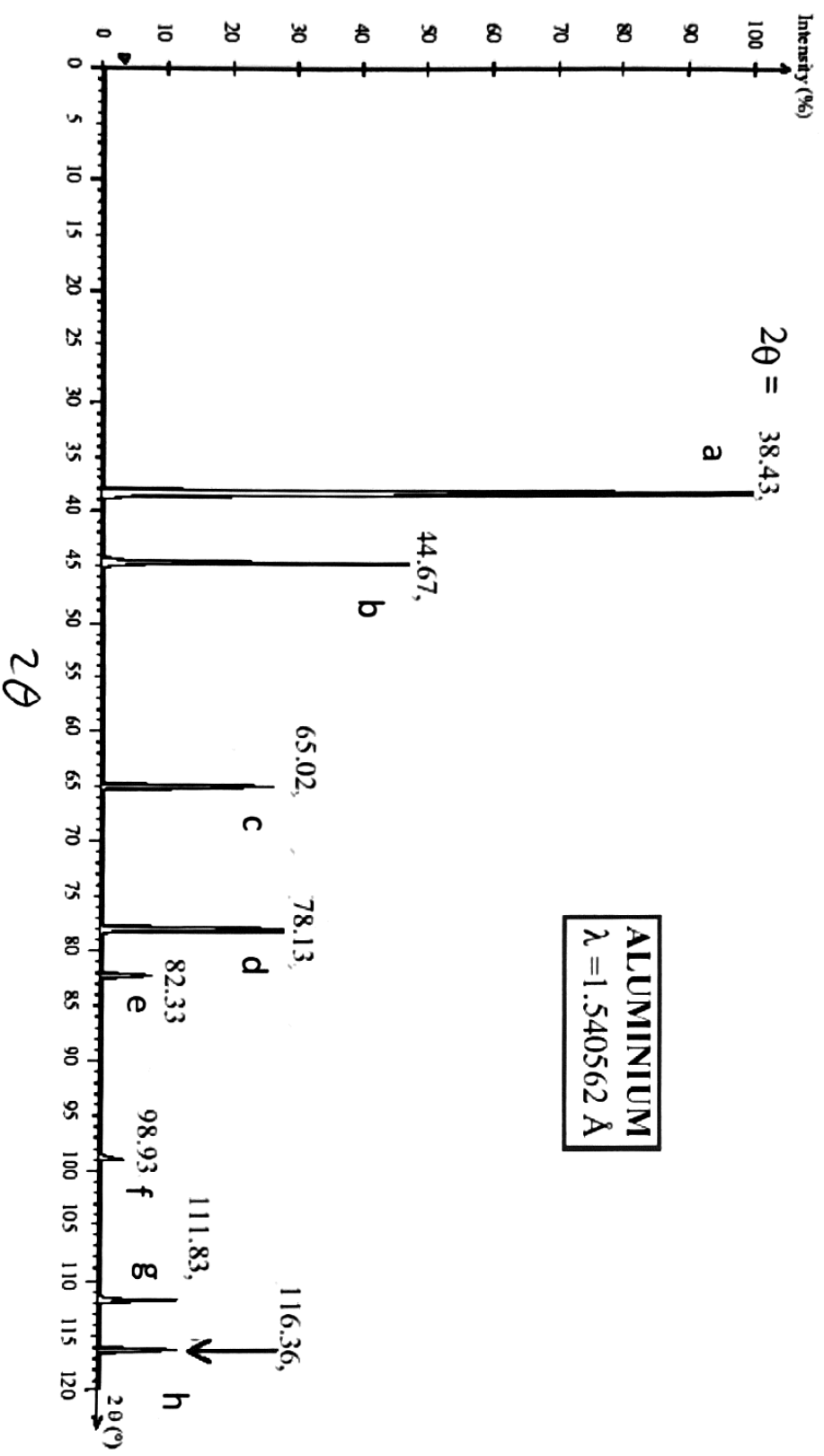$$d = \frac{\lambda}{2 \sin \theta} \qquad \text{assume } n=1$$

3. in this course: assume cubic!

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

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

4. look for integer ratios of N and selection rules

Consider the following XRD pattern for Aluminum, which was collected using CuKα radiation.

$2\theta = 38.43$, a

44.67, b

65.02, c

78.13, d

82.33 e

98.93 f

111.83, g

116.36, h

ALUMINIUM
$\lambda = 1.540562\ \text{Å}$

Intensity (%)

2θ

$2\theta\,(°)$

Peak	2θ	$d=\dfrac{\lambda}{2\sin\theta}$	$\dfrac{d_a^2}{d^2}=\dfrac{(h^2+k^2+\ell^2)}{integer}=\dfrac{N}{int.}$	$3\dfrac{d_a^2}{d^2}$
a	38.43	$2.3405=d_a$	1	3
b	44.67	2.0269	1.3333	3.999
c	65.02	1.4332	2.6667	8.0002
d	78.13	1.2223	3.6666	10.999
e	82.33	1.1702	4.000	12.0001
f	98.93	1.0135	5.3327	'
g	111.83	0.9301	6.3327	
h	116.36	0.09065	6.6657	

$\downarrow$

fcc !