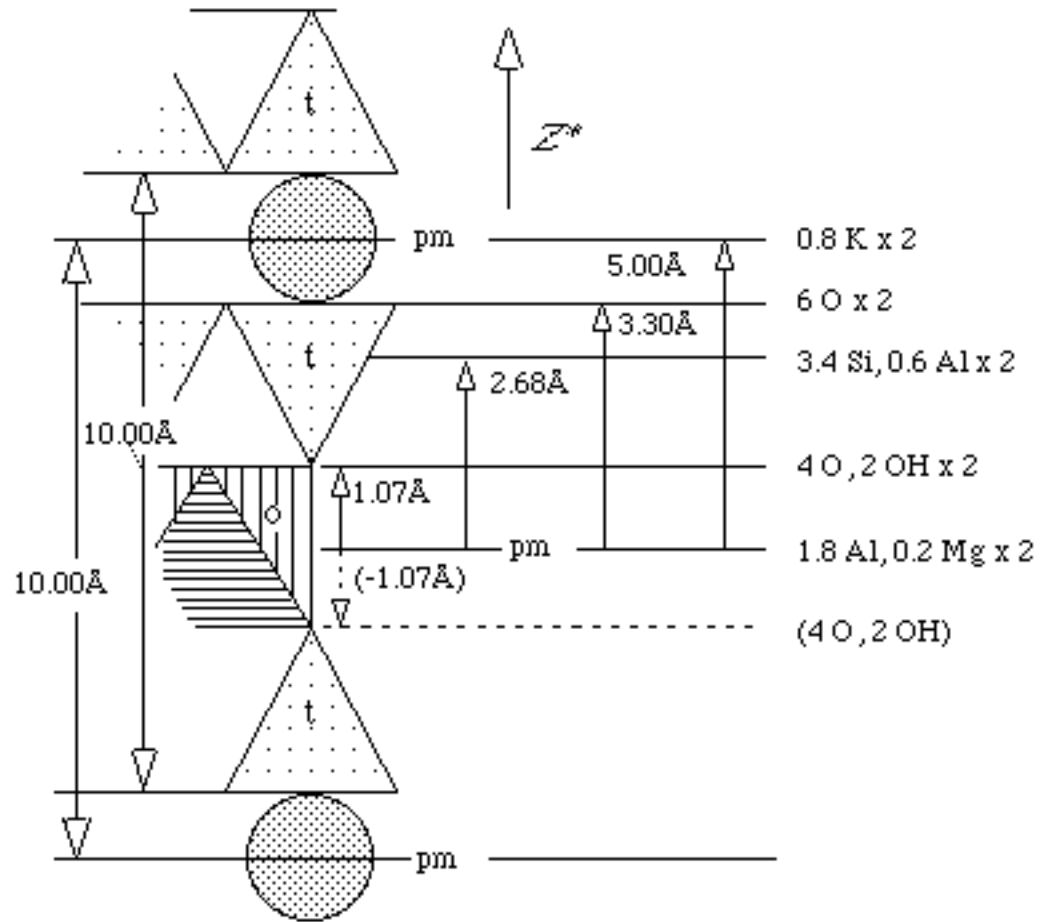
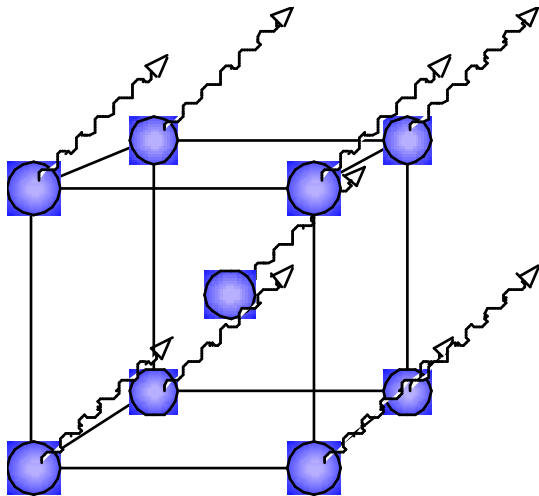


NEWMOD: Calculating XRD patterns



Scientific Revolution??

Copernicus (1473-1543), Galileo (1564 –1642), Kepler (1571 – 1630), Descartes (1596 –1650), Newton Huygens (1629 –1695), Robert Hooke (1635 – 1703), Isaac Newton (1643 –1727), Benjamin Franklin (1706– 1790), Priestley (1733 – 1804), Lavoisier (1743 –1794), Dalton (1766 - 1844), Charles Darwin (1809 – 1882), von Helmholtz (1821 –1894), J.J. Balmer (1825-1898), Edward Morley (1838 - 1923)

Röntgen (1845 – 1923),

Albert Michelson (1852 – 1931), J.J. Thompson (1856–1940), Max Planck (1858 – 1947), W.H. Bragg (1862 –1942), Robert Millikan (1868 – 1953), Rutherford (1871 – 1937), Einstein (1879 – 1955), Max von Laue (1879 - 1960), Niels Bohr (1885 –1962), Henry Moseley (1887 –1915), W.L. Bragg (1890 – 1971), . . . large group of astrophysicists and particle physicists in 21st Century <5% matter as we know it and planets around other suns

Herr Prof. Röntgen



Background, why?

**Why Prof. Roentgen in
1895?**

Why Max von Laue in 1912?

Von Laue, Friedrich, and Knipping's experiment established:

1. Atomic particles within xls are arranged in orderly, 3-D, repeating patterns
2. These regular arrangements have spacings of approximately the same dimensions as the wavelength of X-rays, and
3. X-rays are wave-like in nature.

The Bragg's, W.H. (1862-1942) and W.L. (1890-1971)

Between them, they invited X-ray crystallography

T. Terada 1913

G. Wulff 1913

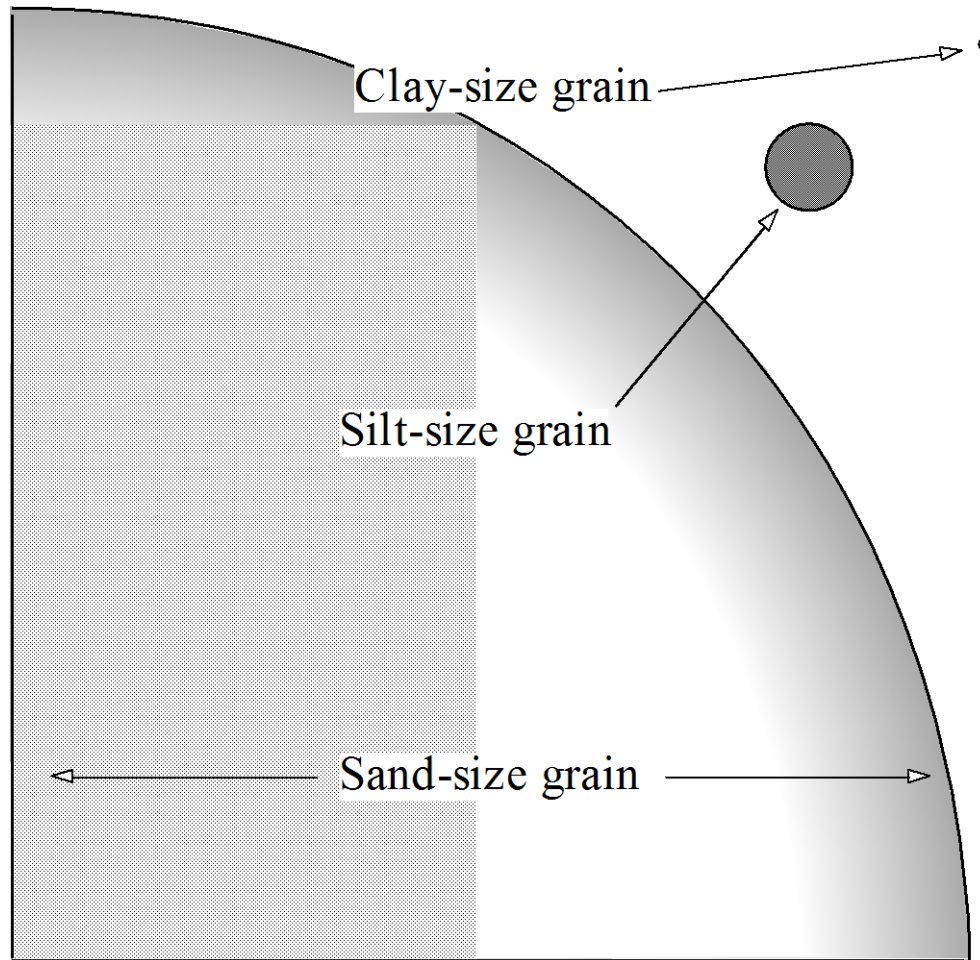
Cascade of crystal structures

J.W. Gruner (1890-1981) and UNM kaolinite in 1932

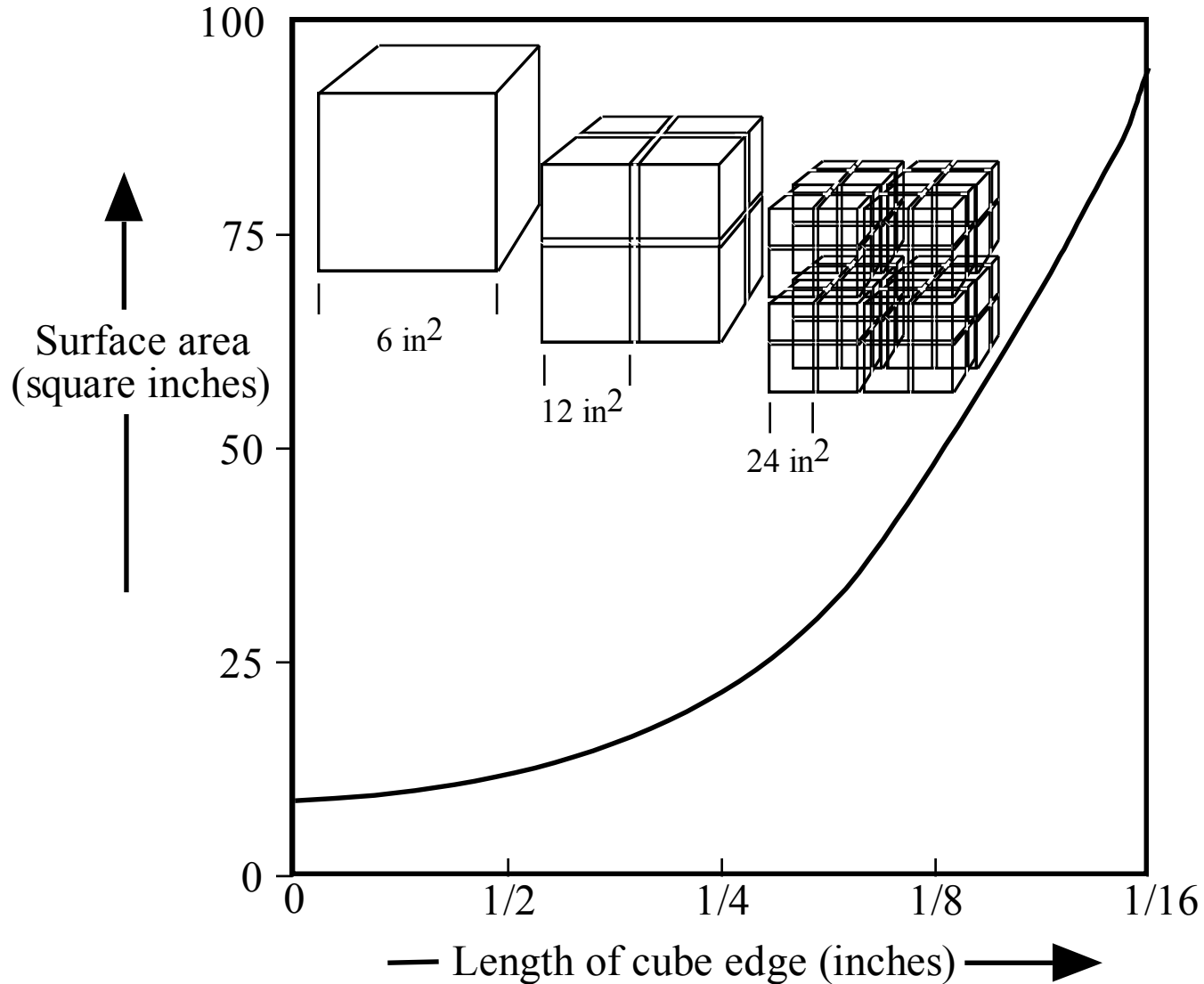
After Pauling (1901 - 1994) published structures of
micas and chlorite in 1930

The Importance of Size

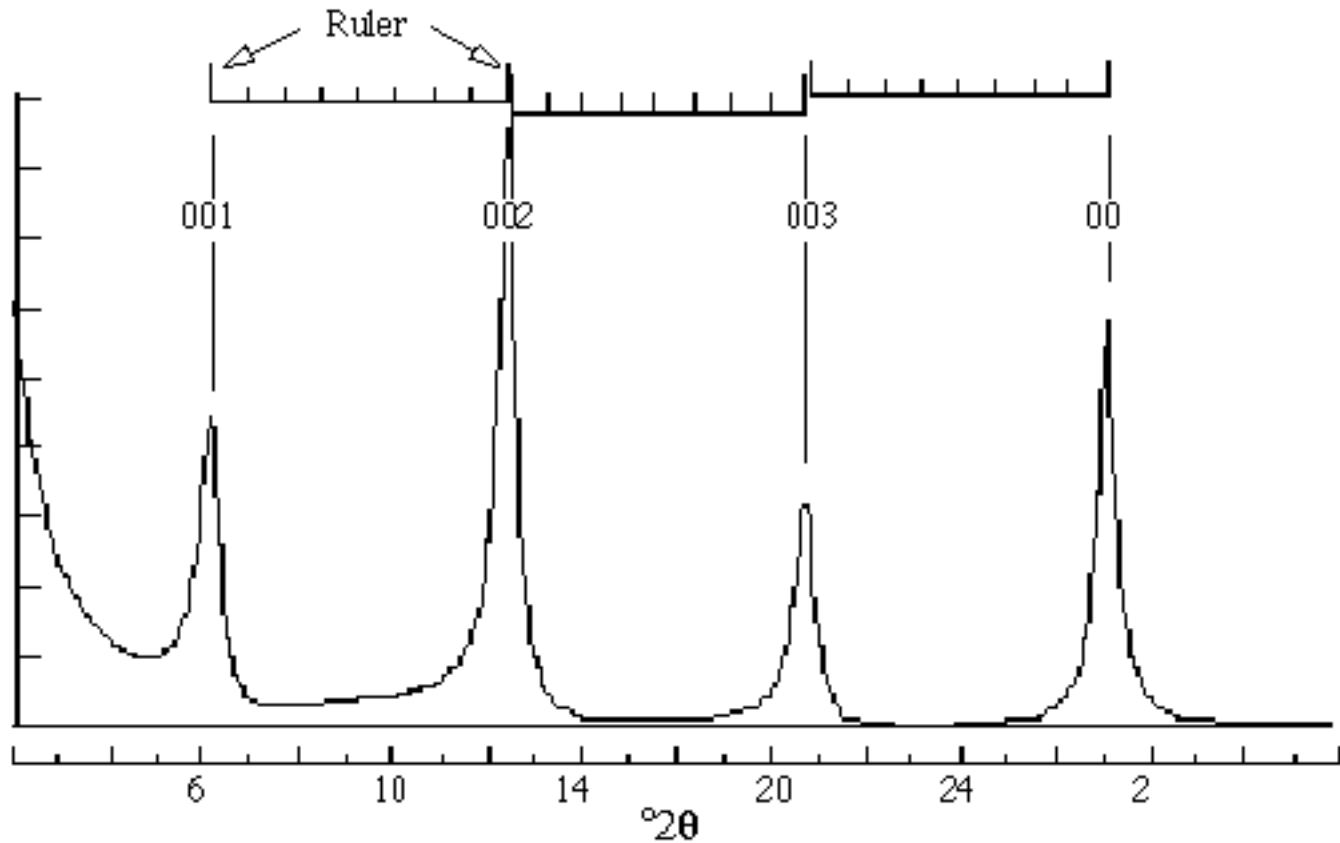
- Limits of abrasion
- Limits of crystallite size (CSD)
- Surface to volume ratio and consequential properties
 - permanent charge
 - reactivity
 - CEC
 - adsorption
 - origin of life
 - plasticity

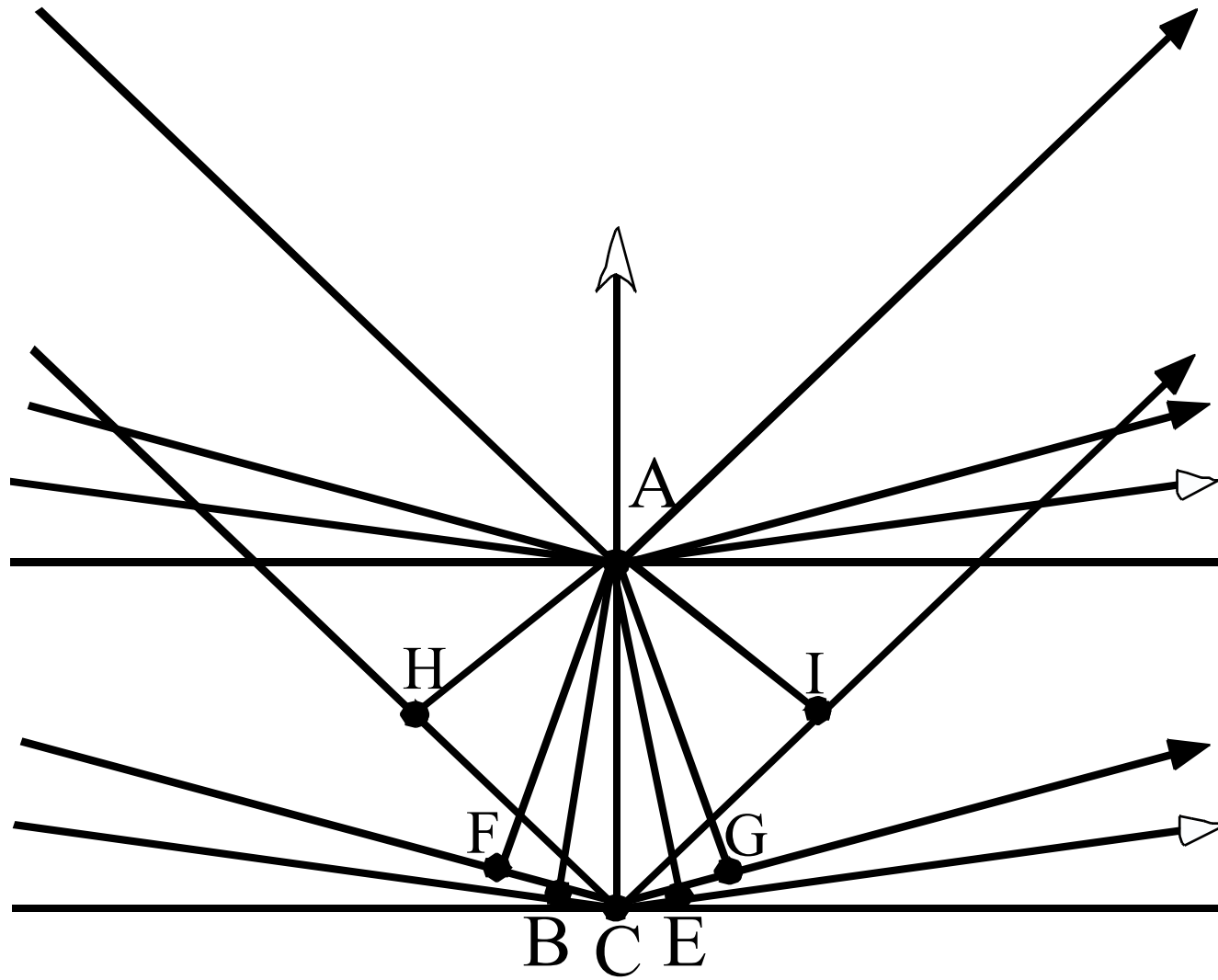


Relation of Particle Size to Surface Area



Why the 00/ diffraction series (chlorite)?



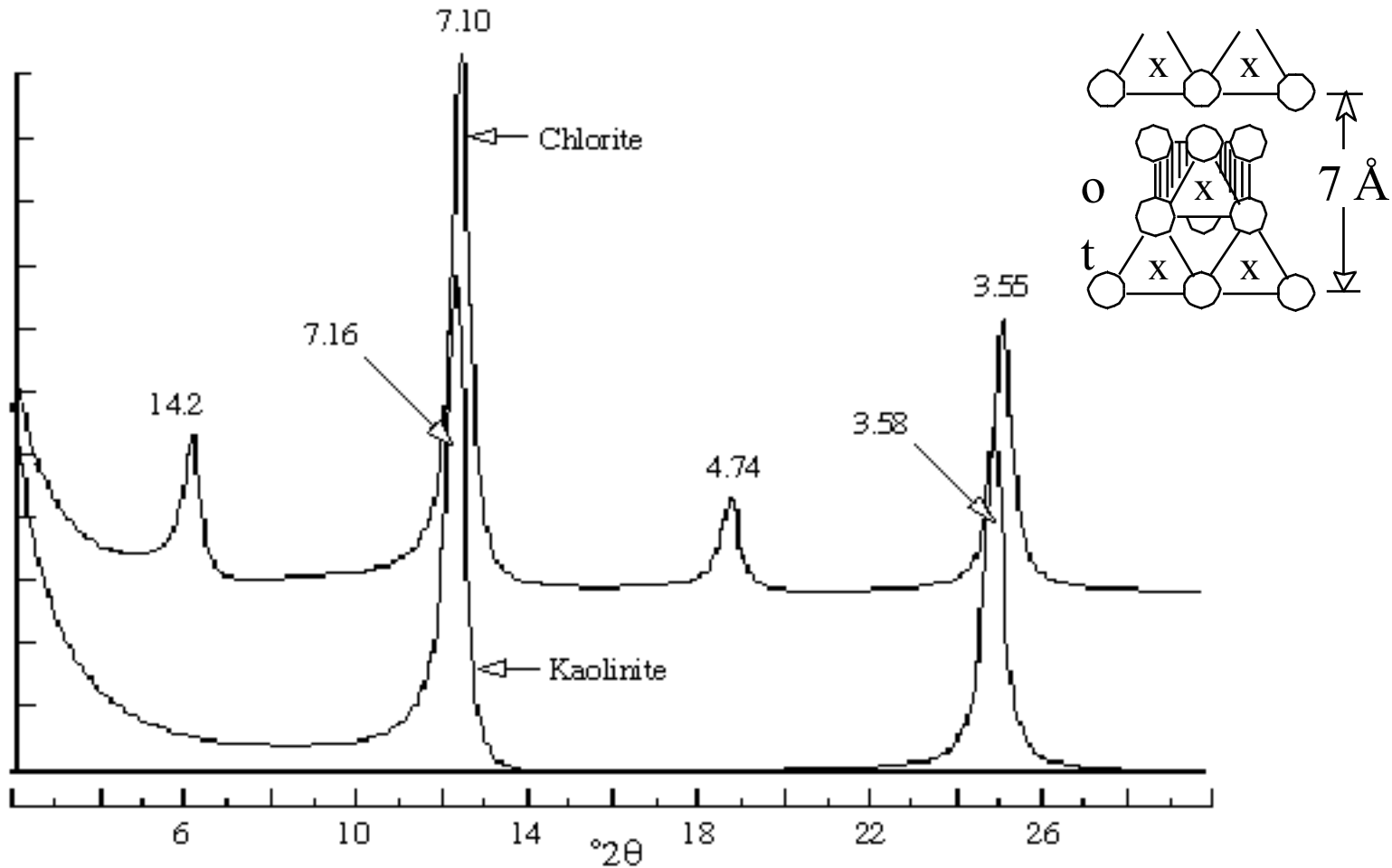


$BC + CE = 1\lambda$ (makes the 001)

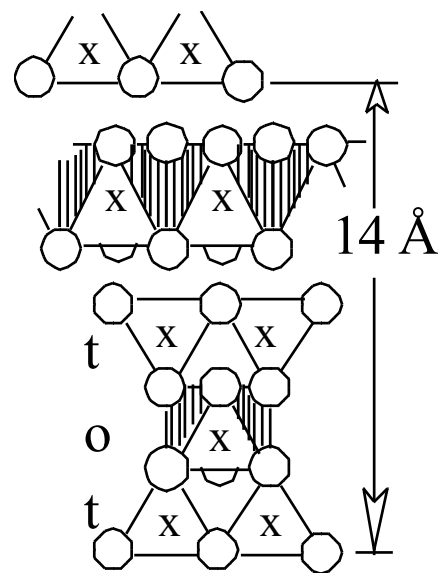
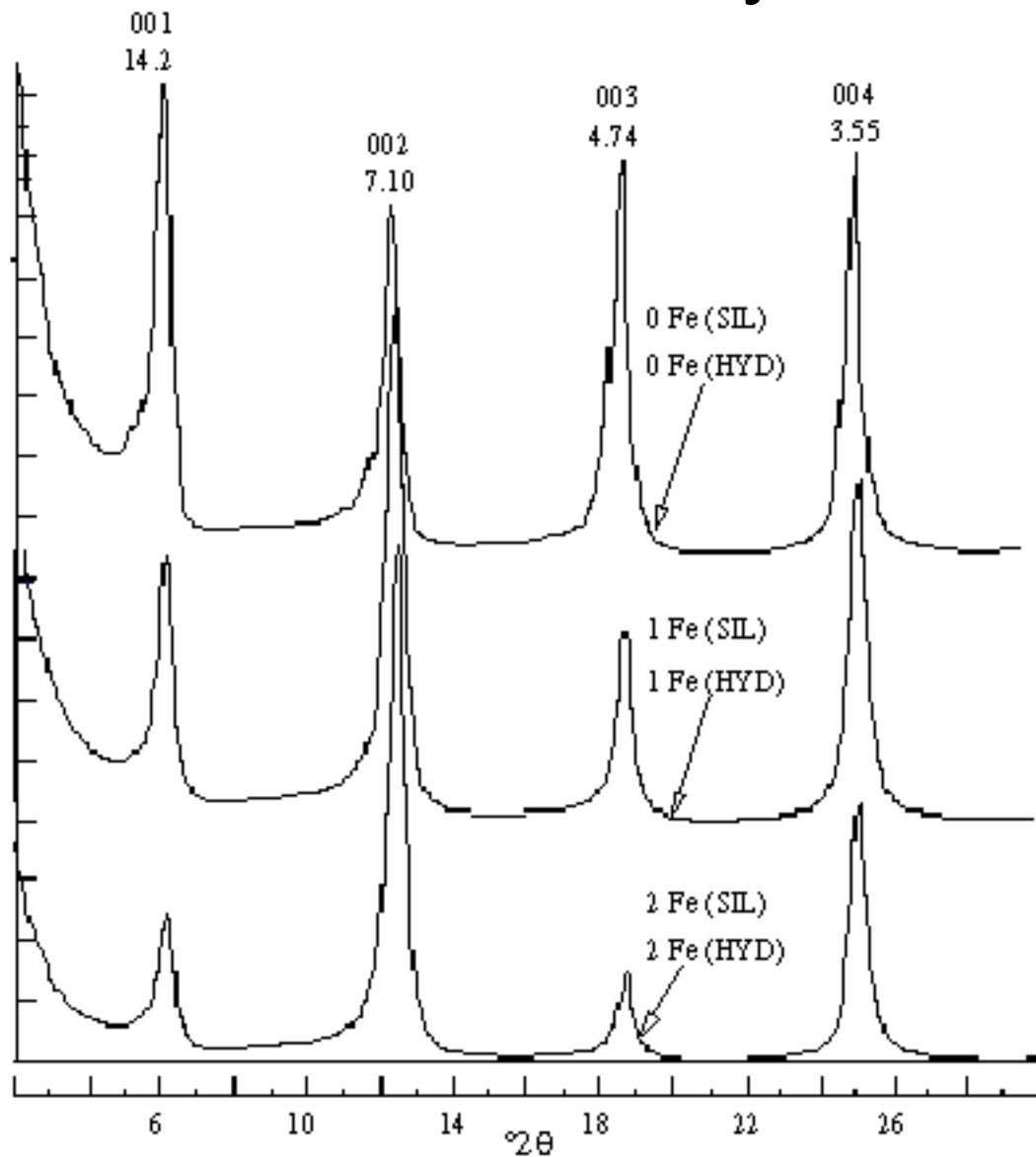
$FC + CG = 2\lambda$ (makes the 002)

$HC + CI = 5\lambda$ (makes the 005)

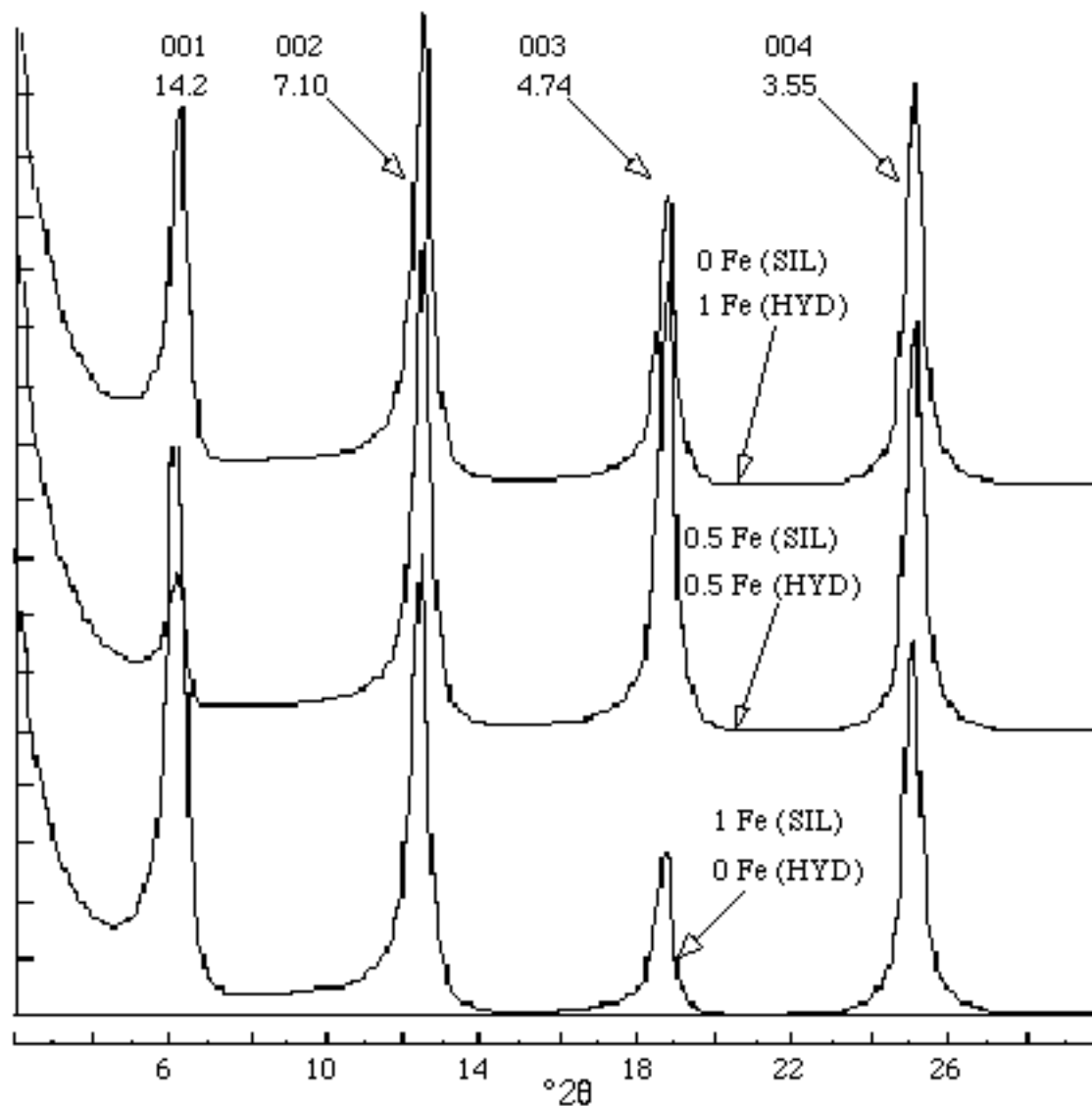
XRD tracks of kao & hi Fe chlorite



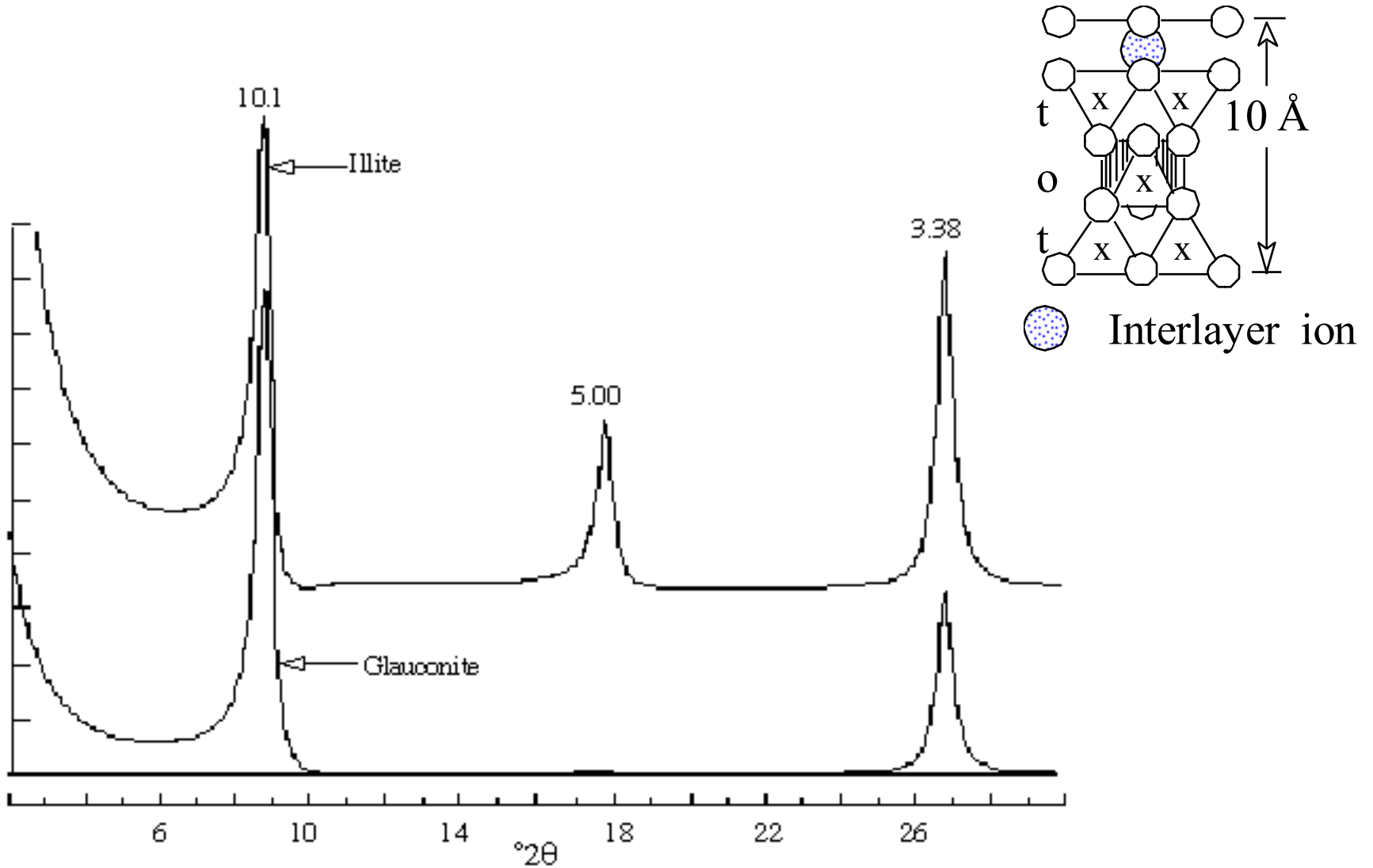
XRD tracks of 'symmetrical' chlorite



XRD track of 'non-symmetrical chlorite



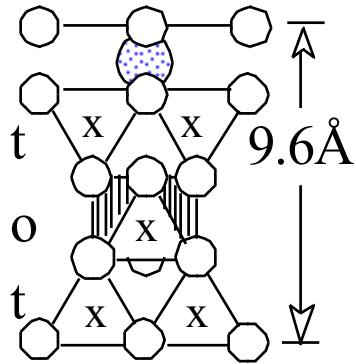
XRD tracks of illite & glauconite



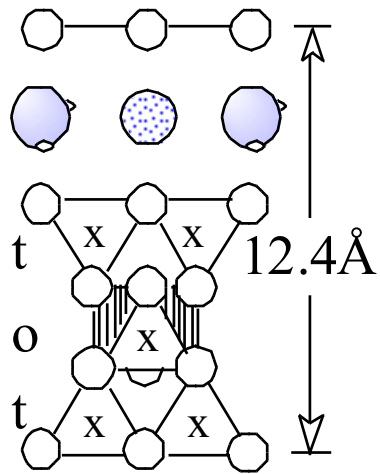
Amazing, expanding smectite

 Interlayer ion

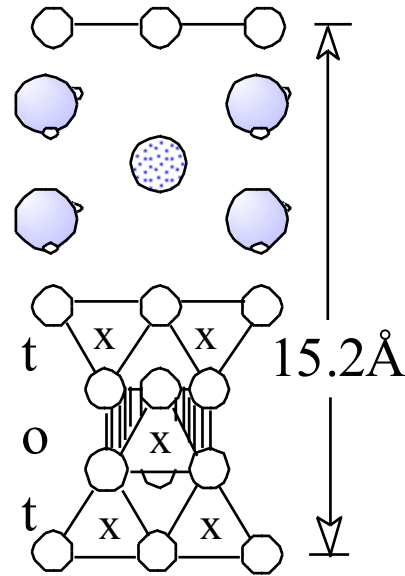
 Water molecule



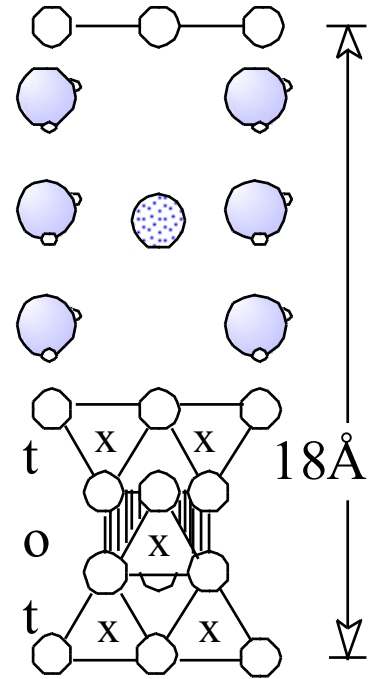
A.



B.

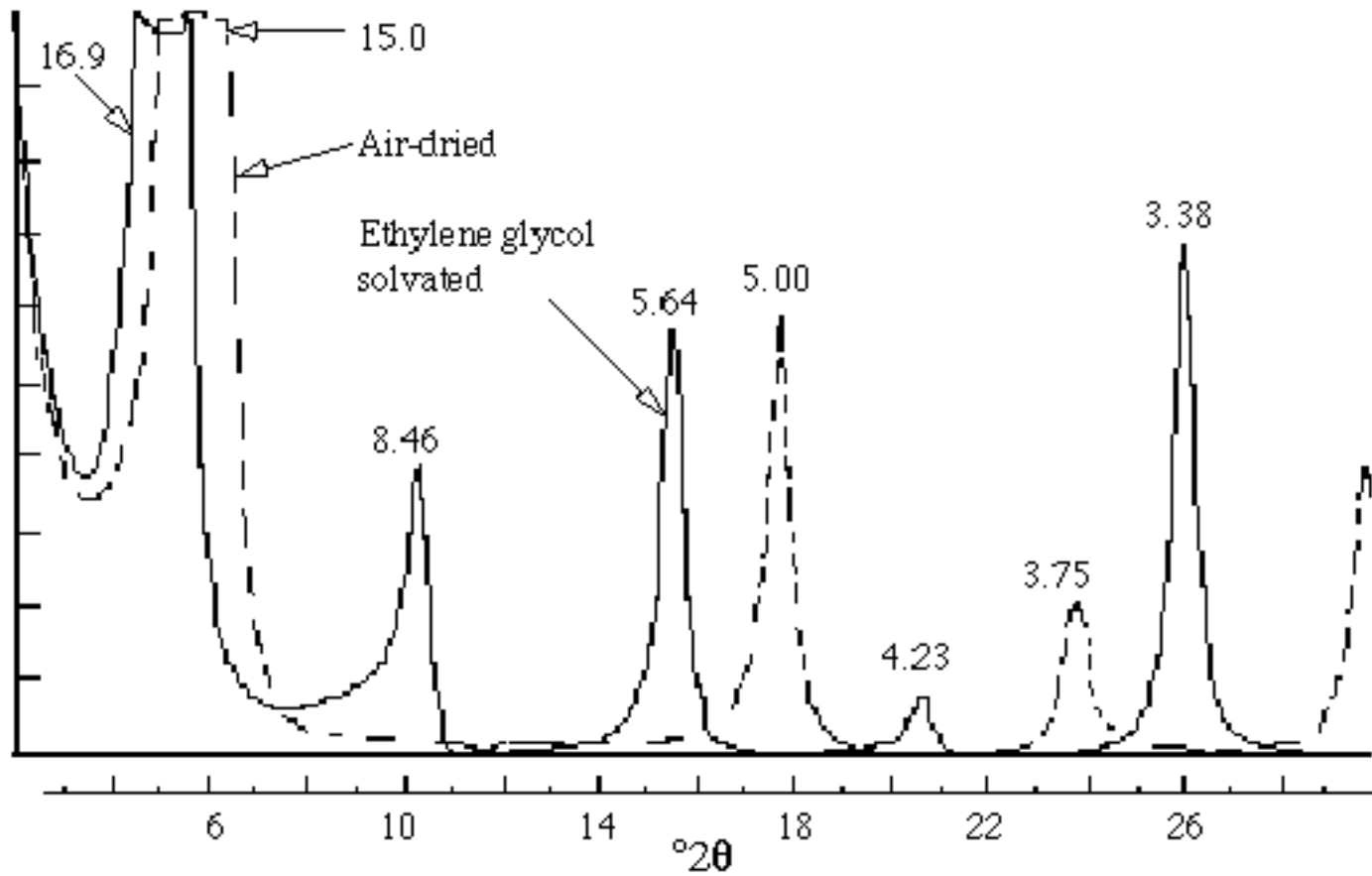


C.

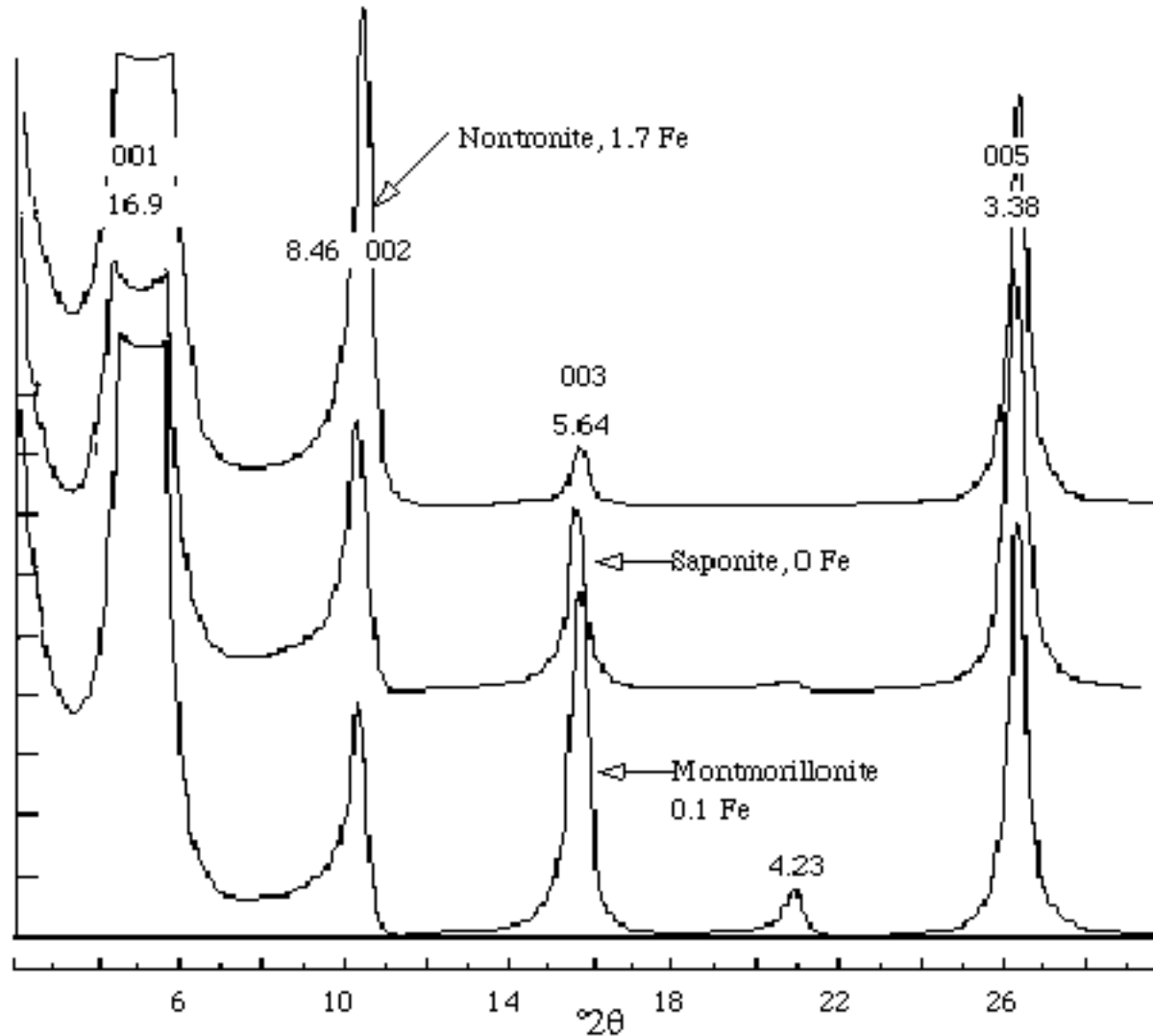


D.

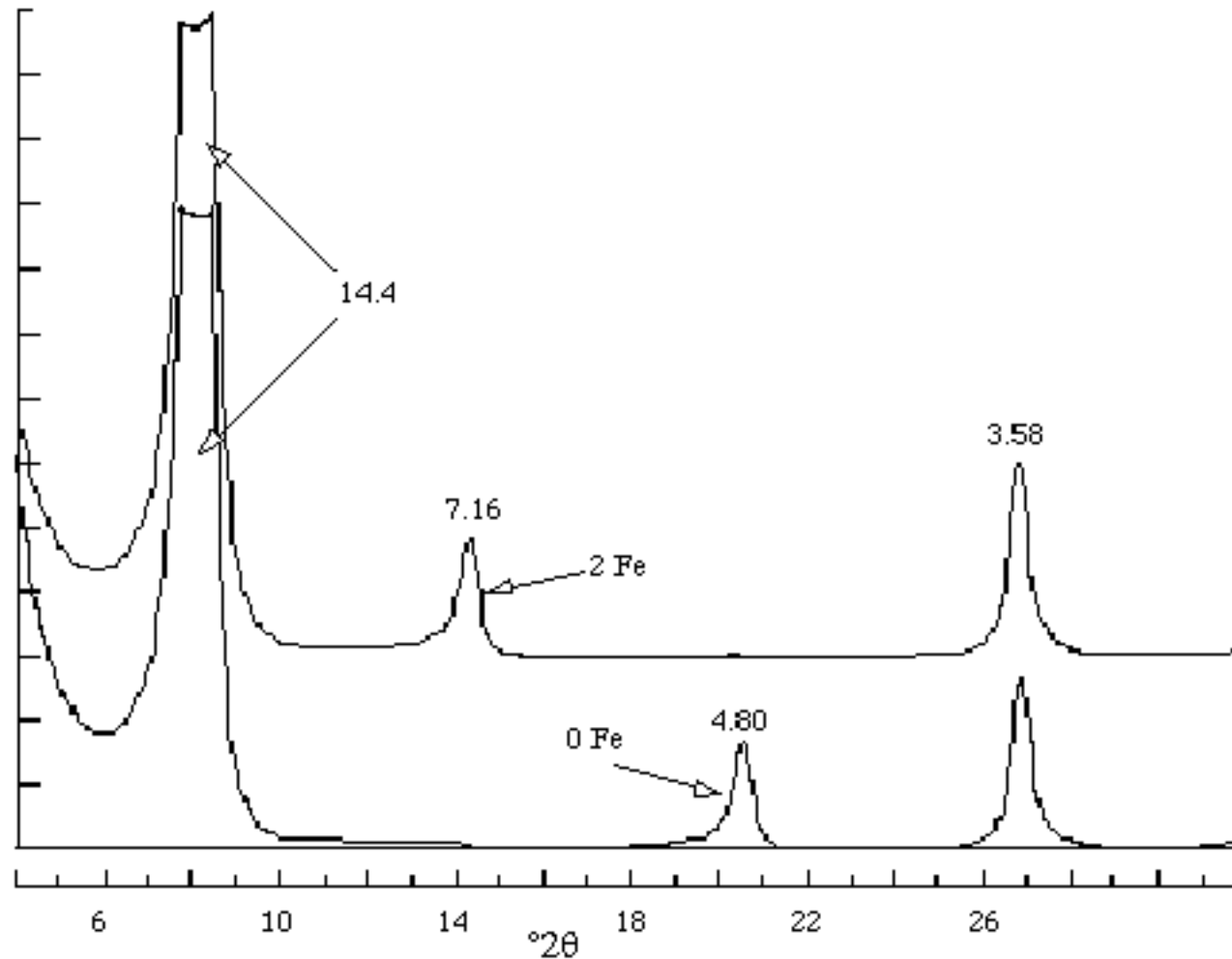
AD & EG XRD tracks of smectite



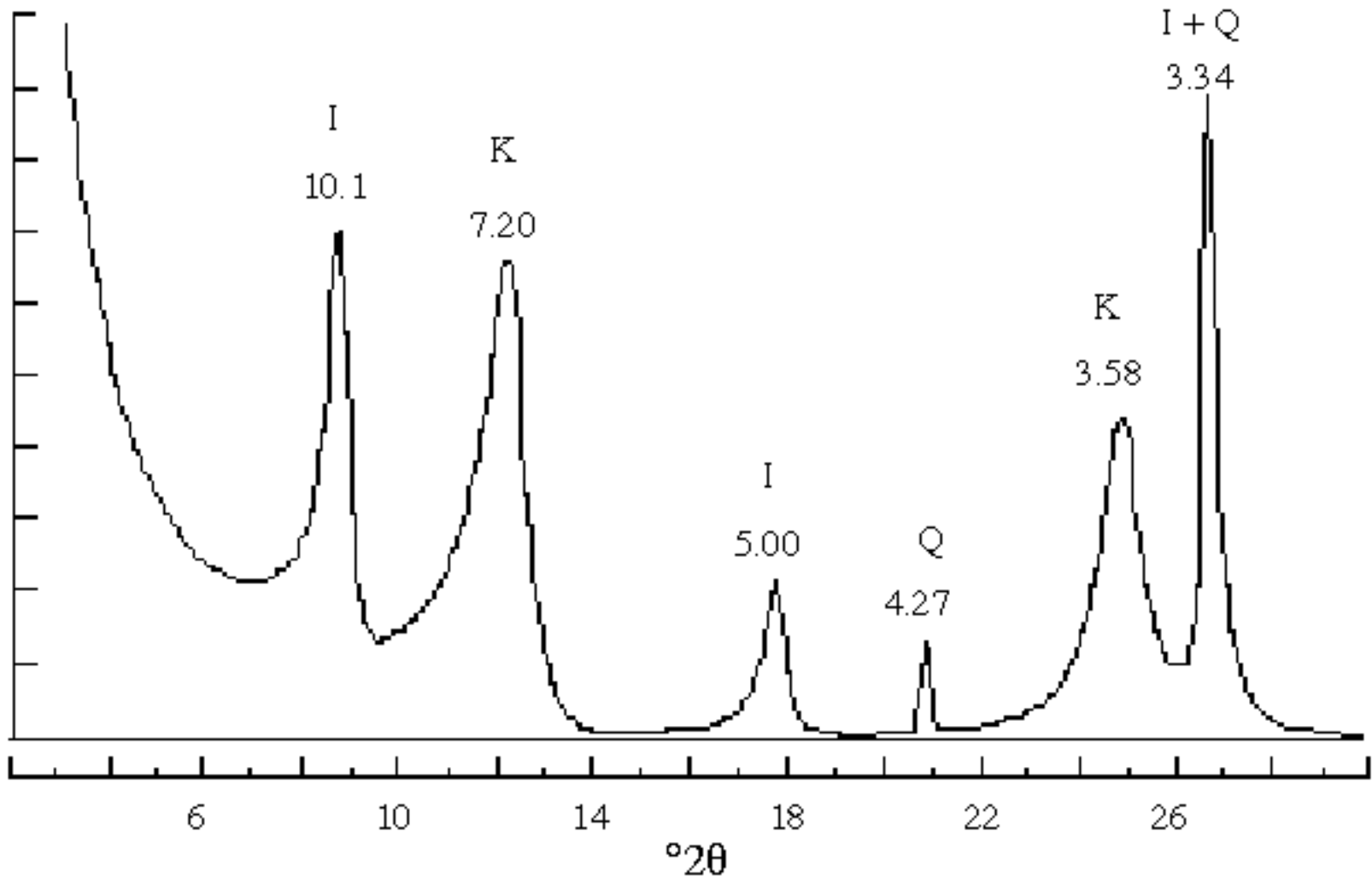
Effects of scattering from octahedral Fe in EG smectites



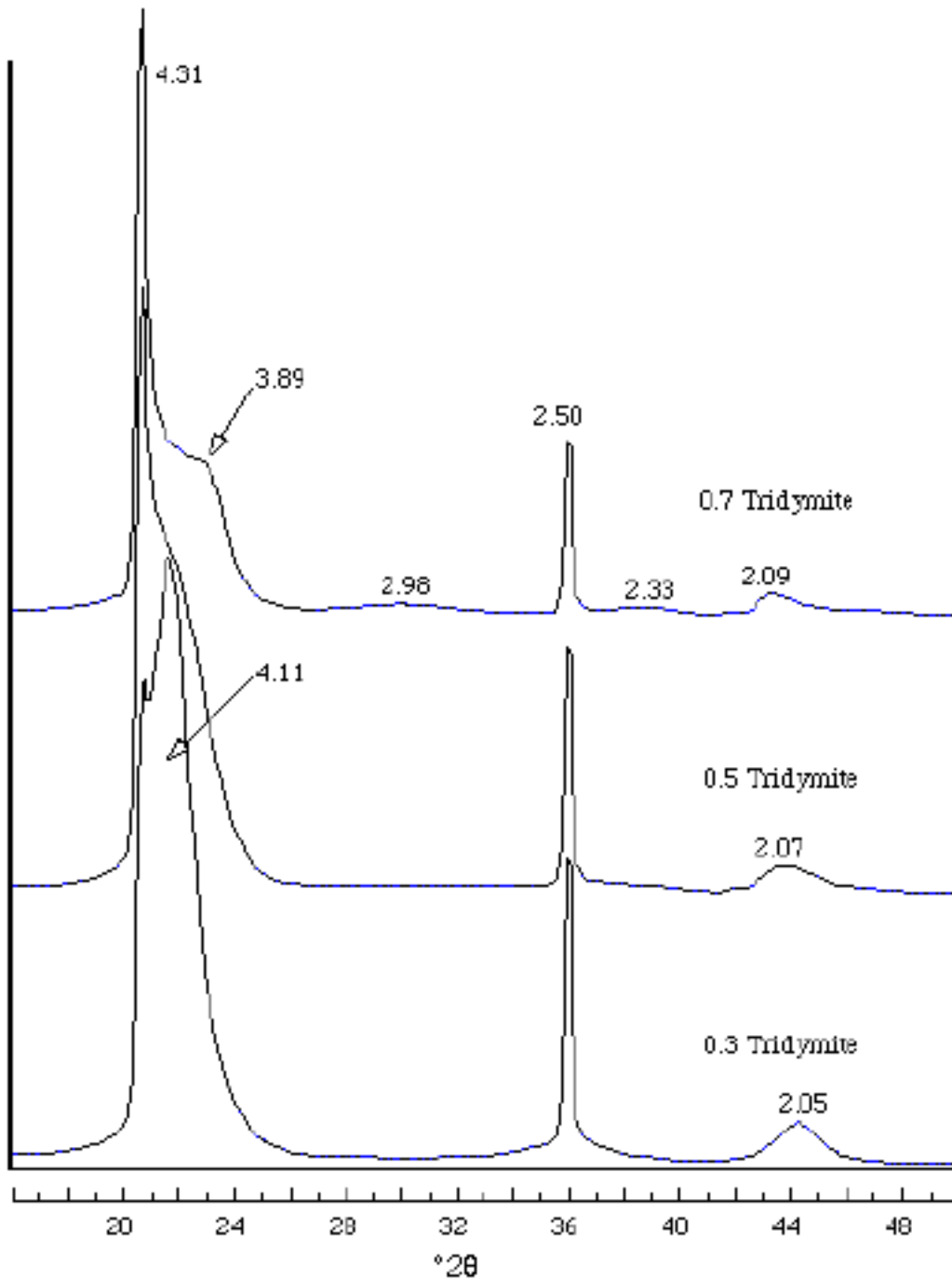
XRD track of AD Mg-vermiculite



A mix of illite, kaolinite & quartz



Calculated patterns, mixed-layered hi-tridymite/hi-cristobalite



1. Evaluation
 - representative?
 - %clay-size material
 - degree of induration

2. Disaggregation
 - crushed not ground

3. Chemical Pretreatments
 - Iron oxides
 - OM
 - cation saturation

4. Size Separation & Dispersion
 - Stokes Law
 - oriented or random

Stokes Law

$$V_T = \frac{g(d_p - d_l)D^2}{18\eta}$$

$$V = h/t$$

$$t = \frac{18\eta h}{g(d_p - d_l)D^2}$$

V_T = final velocity

g = gravitational constant

d_p = density of the particle

d_l = density of the liquid

D^2 = diameter of the particle

η = viscosity of the liquid

h = elevation

t = time

Particle size separations

Settling Times without the Centrifuge

$$16\mu\text{m} = 42 \text{ sec/cm}$$

$$8\mu\text{m} = 3 \text{ min/cm}$$

$$4\mu\text{m} = 12 \text{ min/cm}$$

$$2\mu\text{m} = 48 \text{ min/cm}$$

$$1\mu\text{m} = 3 \text{ hr } 10 \text{ min/cm}$$

Centrifuge Times in Min. Assuming Containers Filled to Within 0.5 cm

Specific Gravities

	2.65	2.50	2.20
<Particle size, μm			
2.0@500 RPM	10		
1.0@1000 RPM	11	12	
0.5@2000 RPM		12	
0.1@3500 RPM		95	120
0.05@3750 RPM			450

Table 6.1. Settling times for gravity sedimentation of particles in water at 20° C^a

Diameter (μm)	h(cm)	min	sec
50	—	—	22
20	—	2	20
5	—	37	30
2	3	50	

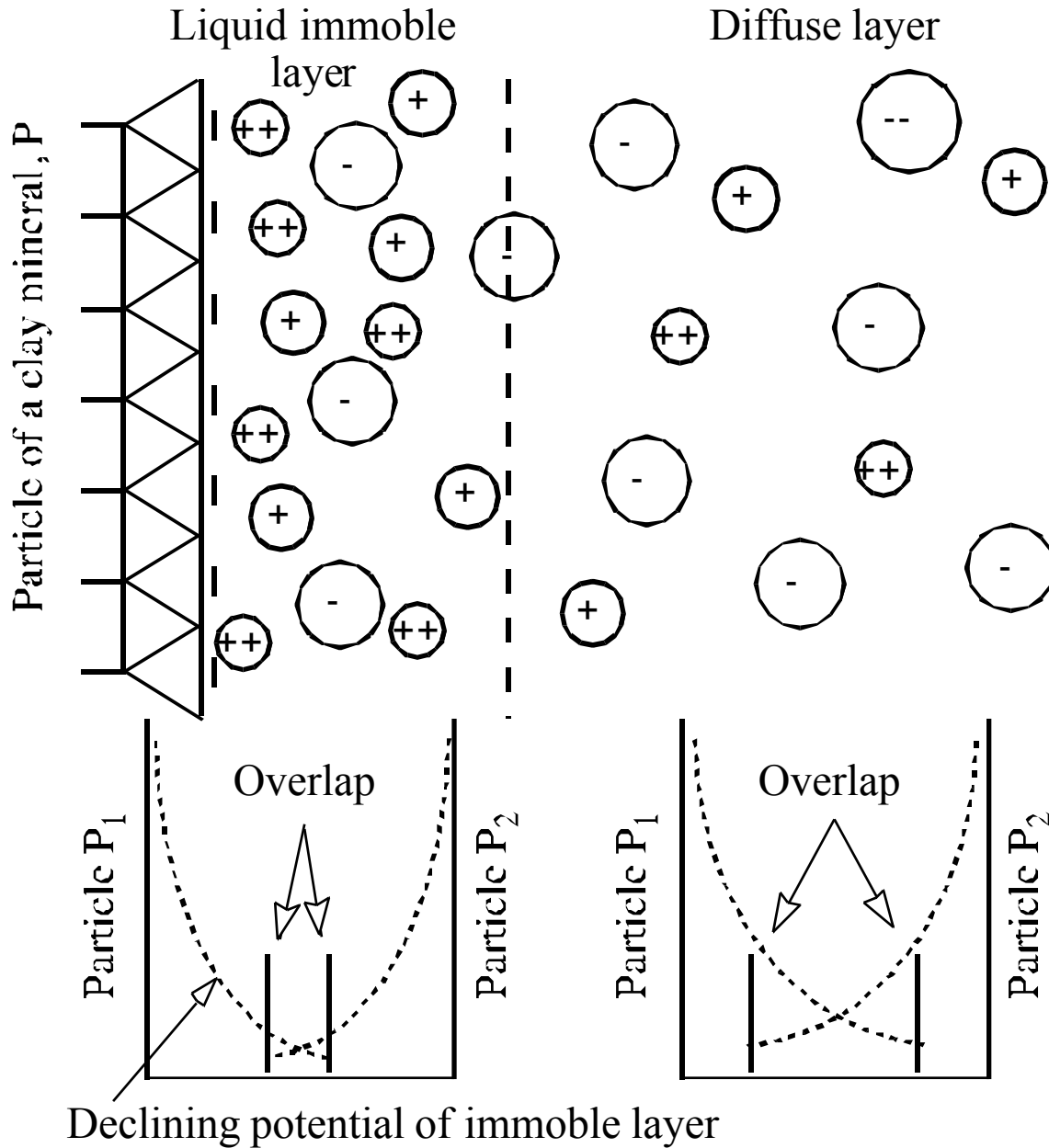
Data apply to a settling distance of 5 cm and a mineral density of 2.65 (Jackson, 1969). ^aThe viscosity of water is a function of temperature.

Table 6.2. Settling times for a specific centrifuge for sedimentation of particles^a

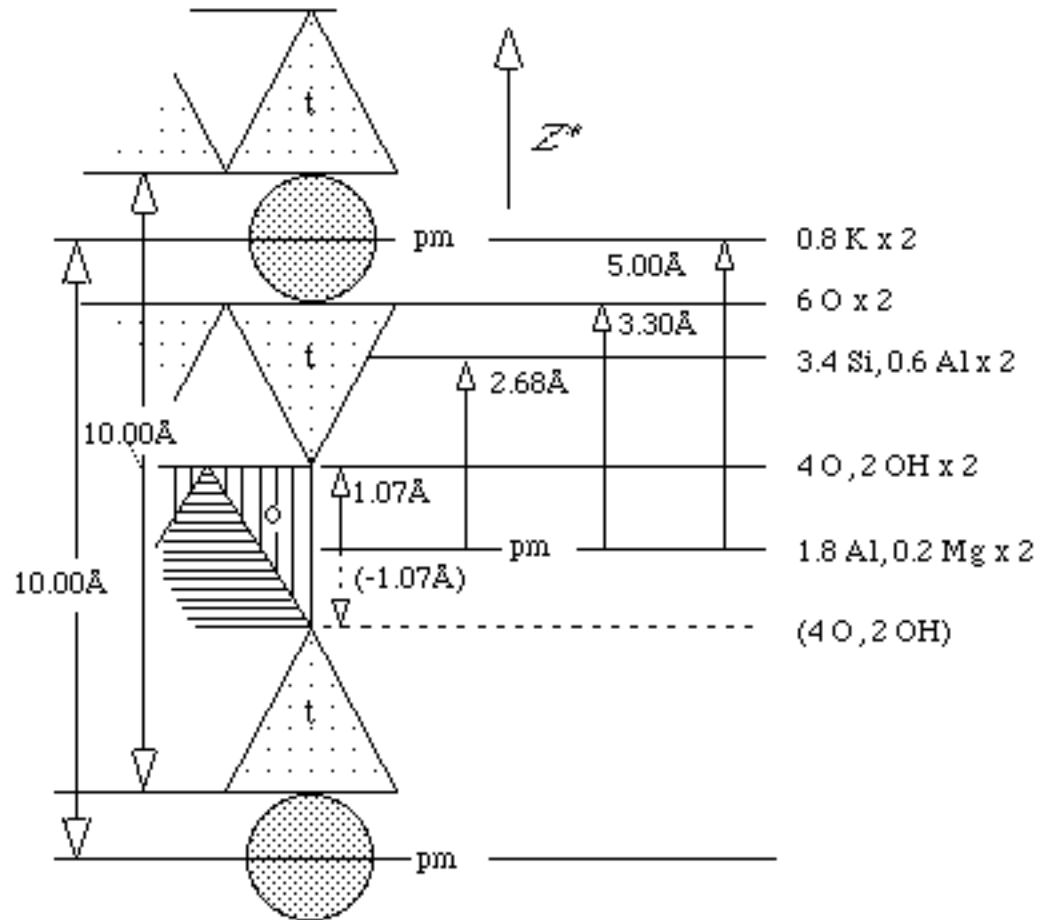
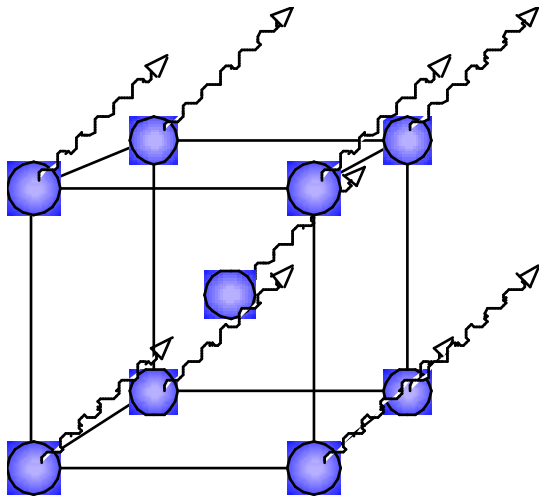
Diameter (μm)	sp. g. mineral	Centrifuge speed (RPM)	time (min)
5	2.65	300	3.3
2	2.65	750	3.3
0.2	2.50	2400	35.4

^aData apply to 20°C, a distance of 15 cm from the centrifuge axis to the liquid meniscus, a 10-cm suspension depth, and 1 cm of sediment at the bottom of the centrifuge tube (Jackson, 1969).

The electric double layer



NEWMOD: Calculating XRD patterns

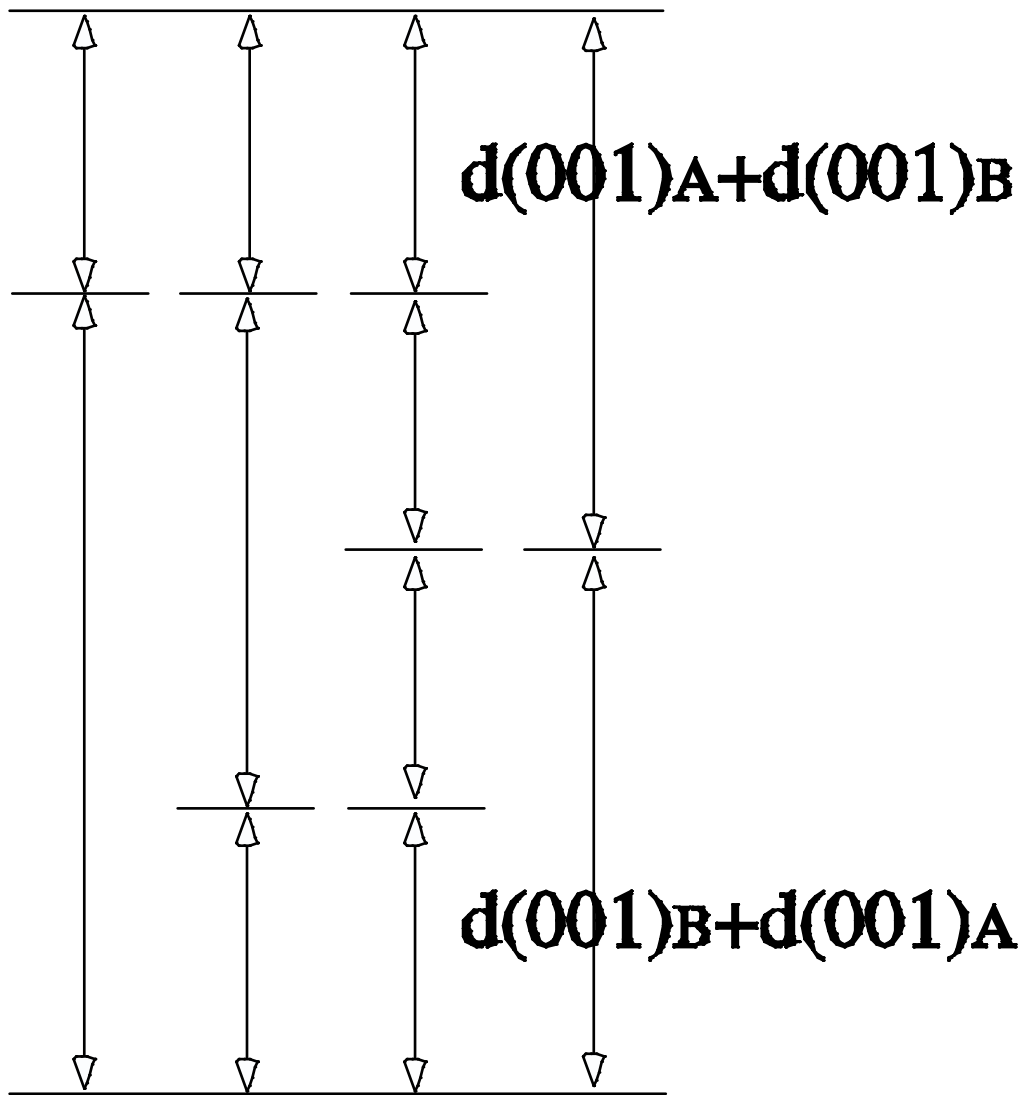
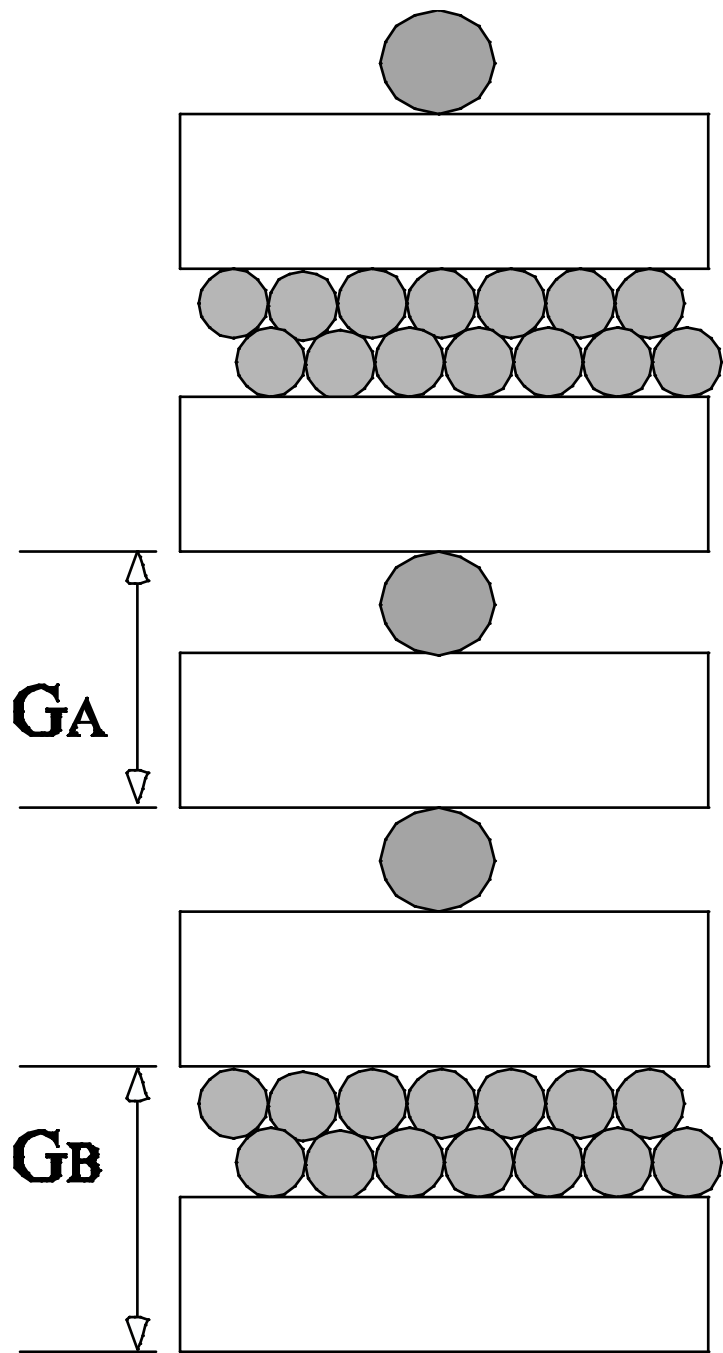


Instrumental variables

Lambda (Cu)	1.5418 Å
Divergence slit	1.0°
Goniometer radius	20 cm
Soller slit 1	6.6°
Soller slit 2	2.0°
Sample length	3.6 cm
Quartz reference intensity	25,000 cps

Default chemical, structural, and sample variables

Exchange capacity	0.35	
Exchange cation		Ca
Fe atoms per 2 or 3 octahedral sites		0-2, 0-3
K per 12-fold site		0-1
Interlayer complex	1-water, 2-glycol, etc.	
μ^* (mass absorption coefficient)	45	
σ^* (std dev of orientation)		12
Low N	3	
High N	14	
$q(N)$ xllite size distribution	1	
δ	variable	
Proportion of component in mixed-layering		0-1
Reichweite (only in mixed-layering)	0, 1, 2, 3	



Reichweite = the reach back

$$P_A + P_B = 1$$

$$[P_{A.B} = 1 \text{ and } P_{A.A} = 0] = R1$$

If $P_B = 0.7$, then, if R1, $P_{A.A} = ?$

$$P_{A.A.A.B} = R3$$

Summing the scattering

