95.545 Sept. 17, 2009 Meg Ann Noah

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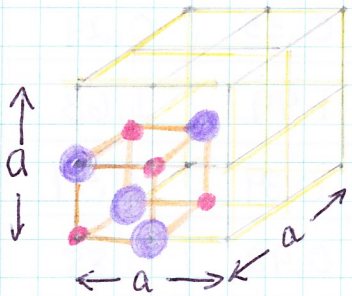
NaCl Unit Cell



fractional x, y, z of cubic (simple)

1	Na	(0, 0, 0)
2	Na	(½, ½, 0)
3	Na	(½, 0, ½)
4	Na	(0, ½, ½)
5	Cl	(0, 0, ½)
6	Cl	(½, ½, ½)
7	Cl	(½, 0, 0)
8	Cl	(0, ½, 0)

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a) Structure Factor: $(e^{-ix} = \cos x - i\sin x)$

$$S(h,k,l) = \sum_{j=1}^{natom} f_j \exp\{-i2\pi(hx_j + ky_j + lz_j)$$

$$= f_{Na}\{1 + e^{-2\pi i(h/2+k/2)} + e^{-2\pi i(h/2+l/2)} + e^{-2\pi i(k/2+l/2)}\}$$

$$+ f_{Cl}\{e^{-i\pi h} + e^{-i\pi k} + e^{-i\pi l} + e^{-i\pi(h+k+l)}\}$$

b) $S(100) = f_{Na}\{1 + e^{-i\pi} + e^{-i\pi} + 1\} + f_{Cl}\{e^{-i\pi} + 1 + 1 + e^{-i\pi}\} = f_{Na}(1-1-1+1) + f_{Cl}(-1+1+1-1) = 0$

$S(110) = f_{Na}\{1 + e^{-2i\pi} + e^{-i\pi} + e^{-i\pi}\} + f_{Cl}\{e^{-i\pi} + e^{-i\pi} + 1 + e^{-2i\pi}\} = 0$

$S(210) = f_{Na}\{1 + e^{-3i\pi} + e^{-2i\pi} + e^{-i\pi}\} + f_{Cl}\{e^{-i\pi 2} + e^{-i\pi} + 1 + e^{-i\pi 3}\} = 0$

c) Calculate in terms of f_{Cl} and f_{Na}

$S(111) = f_{Na}\{1 + e^{-2\pi i} + e^{-2\pi i} + e^{-2\pi i}\} + f_{Cl}\{e^{-i\pi} + e^{-i\pi} + e^{-i\pi} + e^{-3i\pi}\} = 4f_{Na} - 4f_{Cl}$

$S(200) = f_{Na}\{1 + e^{-2\pi i} + e^{-2\pi i} + 1\} + f_{Cl}\{e^{-2i\pi} + 1 + 1 + e^{-2i\pi}\} = 4f_{Na} + 4f_{Cl}$

$S(220) = f_{Na}\{1 + e^{-4\pi i} + e^{-2\pi i} + e^{-2\pi i}\} + f_{Cl}\{e^{-i2\pi} + e^{-i2\pi} + e^{-i2\pi} + e^{-i4\pi}\} = 4f_{Na} + 4f_{Cl}$

$S(222) = f_{Na}\{1 + e^{-4\pi i} + e^{-4\pi i} + e^{-4\pi i}\} + f_{Cl}\{e^{-i2\pi} + e^{-i2\pi} + e^{-i2\pi} + e^{-i6\pi}\} = 4f_{Na} + 4f_{Cl}$

d) Using $a = 5.64\text{Å}$ and $\lambda = 1.54056\text{Å}$

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

$f_{Cl} = \frac{17}{18} \cdot \sin\theta/\lambda$

$f_{Na} = \frac{11}{10} \sin\theta/\lambda$

$$LP = \frac{(1 + \cos^2 2\theta)}{(8\cos\theta\sin^2\theta)}$$

Multiplicity:

$M_{n\,0\,0} = 6$
$M_{n\,n\,0} = 12$
$M_{n\,n\,n} = 8$
$M_{n\,n\,2n} = 24$
$M_{n\,n\,n} = 8$
$M_{n\,n\,2n} = 24$
$M_{n\,2n\,3n} = 48$

→

Peak Intensity of X-Ray Powder Diffraction NaCl

	(111)	(200)	(220)	(222)
$(h^2+k^2+l^2)^{-1/2}$	0.58	0.50	0.35	0.29
$d=a(h^2+k^2+l^2)^{-1/2}$ [Å]	3.26	2.82	1.99	1.63
$\sin\theta=\lambda/2d$	0.24	0.27	0.39	0.47
$\cos\theta$	0.97	0.96	0.92	0.88
2θ	27.37°	31.70°	45.45°	56.47°
$\sin\theta/\lambda$(Å)	0.15	0.18	0.25	0.31
f_{Na} [Å^{-1}]	~~1.69~~ 1.5**	~~1.95~~ 1.8	~~2.76~~ 2.5	~~3.38~~ 3.1
f_{Na^+} [Å^{-1}]	~~2.61~~ 2.7	~~3.01~~ 3.24	~~4.26~~ 4.5	~~5.22~~ 5.58
$S(hkl)$	~~6 - 10.3 = -3.69~~ -4.8	~~19.86~~ 20.16	~~28.08~~ 28	~~34.40~~ 34.72
$LP(\theta)$	4.11	3.00	1.36	0.83
$M(hkl)$	8	6	12	8
$I(hkl)=\lvert S(hkl)\rvert^2 \cdot M(hkl) \cdot LP(\theta)$	~~446.79~~ 757.6	~~7703.48~~ 7315.7	~~12825.79~~ 12794.9	~~7829.55~~ 8004.4

** forgot to adjust due to ionization.

* $a = 5.69$ Å $\lambda = 1.54056$ Å

```
function NaClPeakIntensity2
h=2; k=2; l=2;
Lambda = 1.54056;
a = 5.64;
if (h == k & k == l)
   M = 8;
end
if (k == 0 || l == 0)
   M = 12;
end
if (k == 0 && l == 0)
   M = 6;
end
nfNa = 1 + real(exp(-i*pi*(h+k))) + real(exp(-i*pi*(h+l))) + real(exp(-i*pi*(k+l)));
nfCl = real(exp(-i*pi*(h+k+l))) + real(exp(-i*pi*h)) + real(exp(-i*pi*k)) + real(exp(-i*pi*l));
fprintf(1,'\nfactor1=%.2f\n', 1.0/sqrt(h^2+k^2+l^2));
d = a/sqrt(h^2+k^2+l^2); fprintf(1,'d=%.2f\n', d);
Theta = asin(Lambda/(2*d));
fprintf(1,'sin(T)=%.2f\n', Lambda/(2*d));fprintf(1,'cos(T)=%.2f\n', cos(Theta));
fprintf(1,'2T=%.2f\n', 360.0*Theta/pi);fprintf(1,'factor=%.2f\n',sin(Theta)/Lambda);
fNa = 10*sin(Theta)/Lambda;fCl = 8*sin(Theta)/Lambda;
fprintf(1,'fNa=%.2f\n',fNa);fprintf(1,'fCl=%.2f\n',fCl);
S = nfNa*fNa + nfCl*fCl;fprintf(1,'S=%.2f\n',S);
LP = (1.0  + (cos(2*Theta))^2)/(8*cos(Theta)*(sin(Theta))^2);
fprintf(1,'LP=%.2f\n',LP);fprintf(1,'M=%.2f\n',M);fprintf(1,'I=%.2f\n',S*S*M*LP);
```